```
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LOGINID:ssptasjl1626

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2


* * * * * * * * * *   Welcome to STN International   * * * * * * * * * *

 NEWS  1           Web Page for STN Seminar Schedule - N. America
 NEWS  2  JAN 08   CHEMLIST enhanced with New Zealand Inventory of Chemicals
 NEWS  3  JAN 16   CA/CAplus Company Name Thesaurus enhanced and reloaded
 NEWS  4  JAN 16   IPC version 2007.01 thesaurus available on STN
 NEWS  5  JAN 16   WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
 NEWS  6  JAN 22   CA/CAplus updated with revised CAS roles
 NEWS  7  JAN 22   CA/CAplus enhanced with patent applications from India
 NEWS  8  JAN 29   PHAR reloaded with new search and display fields
 NEWS  9  JAN 29   CAS Registry Number crossover limit increased to 300,000 in
                   multiple databases
 NEWS 10  FEB 15   PATDPASPC enhanced with Drug Approval numbers
 NEWS 11  FEB 15   RUSSIAPAT enhanced with pre-1994 records
 NEWS 12  FEB 23   KOREAPAT enhanced with IPC 8 features and functionality
 NEWS 13  FEB 26   MEDLINE reloaded with enhancements
 NEWS 14  FEB 26   EMBASE enhanced with Clinical Trial Number field
 NEWS 15  FEB 26   TOXCENTER enhanced with reloaded MEDLINE
 NEWS 16  FEB 26   IFICDB/IFIPAT/IFIUDB reloaded with enhancements
 NEWS 17  FEB 26   CAS Registry Number crossover limit increased from 10,000
                   to 300,000 in multiple databases
 NEWS 18  MAR 15   WPIDS/WPIX enhanced with new FRAGHITSTR display format
 NEWS 19  MAR 16   CASREACT coverage extended
 NEWS 20  MAR 20   MARPAT now updated daily
 NEWS 21  MAR 22   LWPI reloaded
 NEWS 22  MAR 30   RDISCLOSURE reloaded with enhancements
 NEWS 23  APR 02   JICST-EPLUS removed from database clusters and STN
 NEWS 24  APR 30   GENBANK reloaded and enhanced with Genome Project ID field
 NEWS 25  APR 30   CHEMCATS enhanced with 1.2 million new records
 NEWS 26  APR 30   CA/CAplus enhanced with 1870-1889 U.S. patent records
 NEWS 27  APR 30   INPADOC replaced by INPADOCDB on STN
 NEWS 28  MAY 01   New CAS web site launched
 NEWS 29  MAY 08   CA/CAplus Indian patent publication number format defined
 NEWS 30  MAY 14   RDISCLOSURE on STN Easy enhanced with new search and display
                   fields
 NEWS EXPRESS  NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT
               MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN    Welcome Banner and News Items
 NEWS IPC8     For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that
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* * * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 06:49:26 ON 21 MAY 2007

=> act inc553394/a
THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE
Some commands only work in certain files.  For example, the EXPAND
command can only be used to look at the index in a file which has an
index.  Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of
commands which can be used in this file.

=> fil reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.21       0.21

FILE 'REGISTRY' ENTERED AT 06:49:47 ON 21 MAY 2007
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STRUCTURE FILE UPDATES:   18 MAY 2007  HIGHEST RN 935394-90-4
DICTIONARY FILE UPDATES:  18 MAY 2007  HIGHEST RN 935394-90-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

  Please note that search-term pricing does apply when
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REGISTRY includes numerically searchable data for experimental and
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experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> act inc553394/a
L1              STR
L2          804 SEA FILE=REGISTRY SSS FUL L1

=>
Uploading C:\Program Files\Stnexp\Queries\10553394-interm6B.str

L3      STRUCTURE UPLOADED

=>
Uploading C:\Program Files\Stnexp\Queries\10553394-interm6.str

L4      STRUCTURE UPLOADED

=> s l4 sub=l2 sss full
FULL SUBSET SEARCH INITIATED 06:51:04 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED -       804 TO ITERATE

100.0% PROCESSED      804 ITERATIONS                          727 ANSWERS
SEARCH TIME: 00.00.01
```

```
L5          727 SEA SUB=L2 SSS FUL L4

=> sav tem in6553394/a
ENTER L#, L# RANGE, ALL, OR (END):l5

=> s l3 sub=l2 sss full
FULL SUBSET SEARCH INITIATED 06:51:44 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED -        7 TO ITERATE

100.0% PROCESSED        7 ITERATIONS                                 7 ANSWERS
SEARCH TIME: 00.00.01

L6            7 SEA SUB=L2 SSS FUL L3

=> fil caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                      83.10      83.31

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FILE COVERS 1907 - 21 May 2007  VOL 146 ISS 22
FILE LAST UPDATED: 20 May 2007  (20070520/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l5
L7          236 L5

=> s l6
L8            3 L6

=> d l8 tot bib abs hitstr

L8   ANSWER 1 OF 3  CAPLUS  COPYRIGHT 2007 ACS on STN
AN   2004:902331  CAPLUS
DN   141:379636
TI   Process for preparation of optically active 2-allylcarboxylic acid
     derivatives
IN   Okuro, Kazumi; Amano, Susumu; Kizaki, Noriyuki; Takesue, Teruaki; Mitsuda,
     Masaru; Ito, Noriyuki; Yasohara, Yoshihiko
PA   Kaneka Corporation, Japan; Ono Pharmaceutical Co., Ltd.
SO   PCT Int. Appl., 57 pp.
     CODEN: PIXXD2
DT   Patent
LA   Japanese
FAN.CNT 1
```

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004092113	A1	20041028	WO 2004-JP5465	20040416
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	EP 1650187	A1	20060426	EP 2004-727979	20040416
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
	US 2006223152	A1	20061005	US 2005-553394	20051214
PRAI	JP 2003-114783	A	20030418		
	WO 2004-JP5465	W	20040416		

OS MARPAT 141:379636

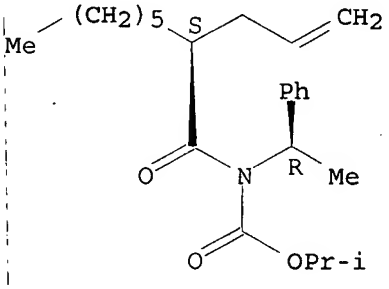
AB This invention pertains to a method for producing optically active 2-allylcarboxylic acid derivs., which comprises preparation of carboxamides, N-allylcarboxamides, rearrangement of allyl group, and hydrolysis processes. For example, (R)- and (S)-2-allyloctanoic acid were prepared starting from (R)-1-phenylethylamine and octanoyl chloride in good yield. This invention provides a method to prepare optically active 2-allylcarboxylic acid derivs. from less expensive starting materials with industrial advantages.

IT 781647-60-7P 781647-61-8P 781647-63-0P
781647-65-2P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of optically active 2-allylcarboxylic acid derivs.)

RN 781647-60-7 CAPLUS

CN Carbamic acid, [(2S)-1-oxo-2-(2-propenyl)octyl][(1R)-1-phenylethyl]-, 1-methylethyl ester (9CI) (CA INDEX NAME)

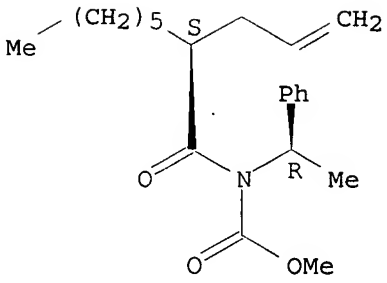
Absolute stereochemistry.



RN 781647-61-8 CAPLUS

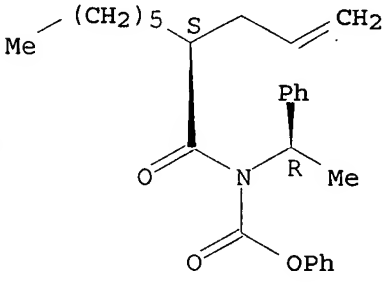
CN Carbamic acid, [(2S)-1-oxo-2-(2-propenyl)octyl][(1R)-1-phenylethyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



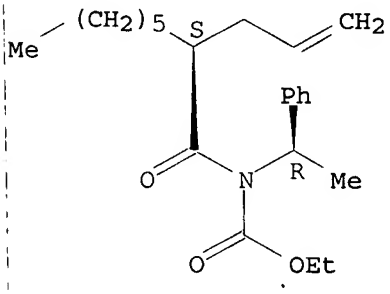
RN 781647-63-0 CAPLUS
CN Carbamic acid, [(2S)-1-oxo-2-(2-propenyl)octyl][(1R)-1-phenylethyl]-, phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



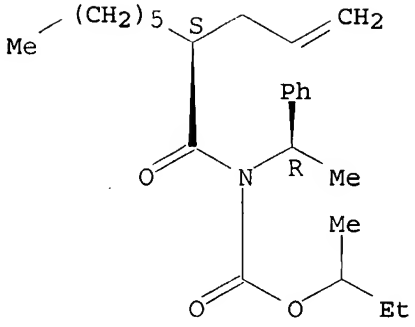
RN 781647-65-2 CAPLUS
CN Carbamic acid, [(2S)-1-oxo-2-(2-propenyl)octyl][(1R)-1-phenylethyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



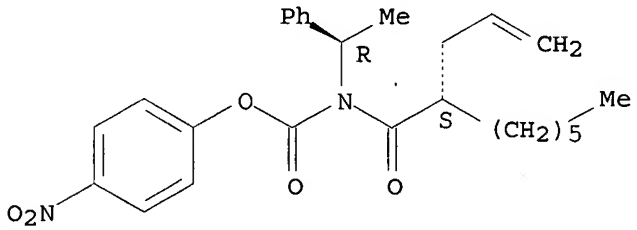
IT 781647-62-9P 781647-64-1P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of optically active 2-allylcarboxylic acid derivs.)
RN 781647-62-9 CAPLUS
CN Carbamic acid, [(2S)-1-oxo-2-(2-propenyl)octyl][(1R)-1-phenylethyl]-, 1-methylpropyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 781647-64-1 CAPLUS
CN Carbamic acid, [(2S)-1-oxo-2-(2-propenyl)octyl][(1R)-1-phenylethyl]-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)

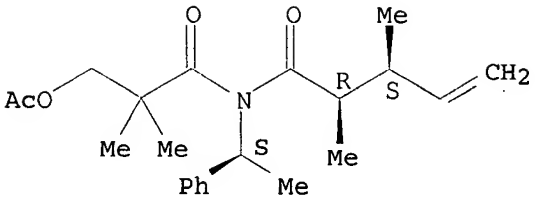
Absolute stereochemistry.



RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

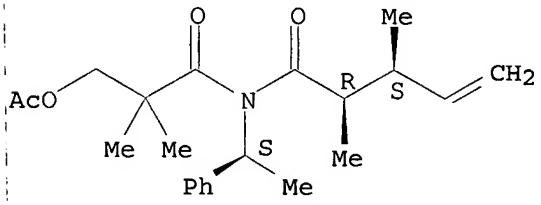
L8 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1992:530592 CAPLUS
DN 117:130592
TI A few new methods toward asymmetric synthesis
AU Ito, Sho; Tsunoda, Tetsuto
CS Fac. Pharm. Sci., Tokushima Bunri Univ., Tokushima, 770, Japan
SO Journal of the Chinese Chemical Society (Taipei, Taiwan) (1992), 39(3), 205-8
CODEN: JCCTAC; ISSN: 0009-4536
DT Journal
LA English
OS CASREACT 117:130592
AB The asym. rearrangement of N-2-butenyl-N-alkylcarboxamides was studied. Thus, treatment of (E)-EtCONBuCH2CH=CHMe with LDA in THF at -78°, followed by exchange of the solvent with xylene gave predominantly syn-CH2:CHCHMeCHMeCONHBu. The latter was hydrolyzed to the acid via the N-acetoxypivaloyl derivative
IT 141447-13-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 141447-13-4 CAPLUS
CN 4-Pentenamide, N-[3-(acetyloxy)-2,2-dimethyl-1-oxopropyl]-2,3-dimethyl-N-(1-phenylethyl)-, [2R-[1(S*),2R*,3S*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1992:255275 CAPLUS
DN 116:255275
TI Asymmetric induction in aza-Claisen rearrangement of carboxamide enolates. Effect of chiral auxiliary on nitrogen
AU Tsunoda, Tetsuto; Sakai, Mika; Sasaki, Osamu; Sako, Yoshie; Hondo, Yuka; Ito, Sho
CS Fac. Pharm. Sci., Tokushima Bunri Univ., Tokushima, 770, Japan
SO Tetrahedron Letters (1992), 33(12), 1651-4
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
OS CASREACT 116:255275
AB Aza-Claisen rearrangement of enolates of N-alkyl-N-(2E)-butenylpropanamides with chiral alkyl groups proceeded with high relative asym. induction as well as excellent internal asym. induction to give optically active N-alkyl-syn-2,3-dimethylpent-4-enamides.
IT 141447-13-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
RN 141447-13-4 CAPLUS
CN 4-Pentenamide, N-[3-(acetyloxy)-2,2-dimethyl-1-oxopropyl]-2,3-dimethyl-N-(1-phenylethyl)-, [2R-[1(S*),2R*,3S*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> fil stng

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	16.28	99.59

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.34	-2.34

FILE 'STNGUIDE' ENTERED AT 06:52:38 ON 21 MAY 2007

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: May 18, 2007 (20070518/UP).

```
=> d his

     (FILE 'HOME' ENTERED AT 06:49:26 ON 21 MAY 2007)

     FILE 'REGISTRY' ENTERED AT 06:49:47 ON 21 MAY 2007
               ACT INC553394/A
              ---------
L1             STR
L2          804 SEA FILE=REGISTRY SSS FUL L1
              ---------
L3             STRUCTURE UPLOADED   interm 6B.str
L4             STRUCTURE UPLOADED   interm 6.str
L5          727 S L4 SSS FULL SUB=L2
               SAV TEM IN6553394/A L5
L6            7 S L3 SSS FULL SUB=L2

     FILE 'CAPLUS' ENTERED AT 06:51:56 ON 21 MAY 2007
L7          236 S L5
L8            3 S L6

     FILE 'STNGUIDE' ENTERED AT 06:52:38 ON 21 MAY 2007

=> log hold
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY    SESSION
FULL ESTIMATED COST                                    0.18      99.77

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                      ENTRY    SESSION
CA SUBSCRIBER PRICE                                    0.00      -2.34

 SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 06:54:10 ON 21 MAY 2007
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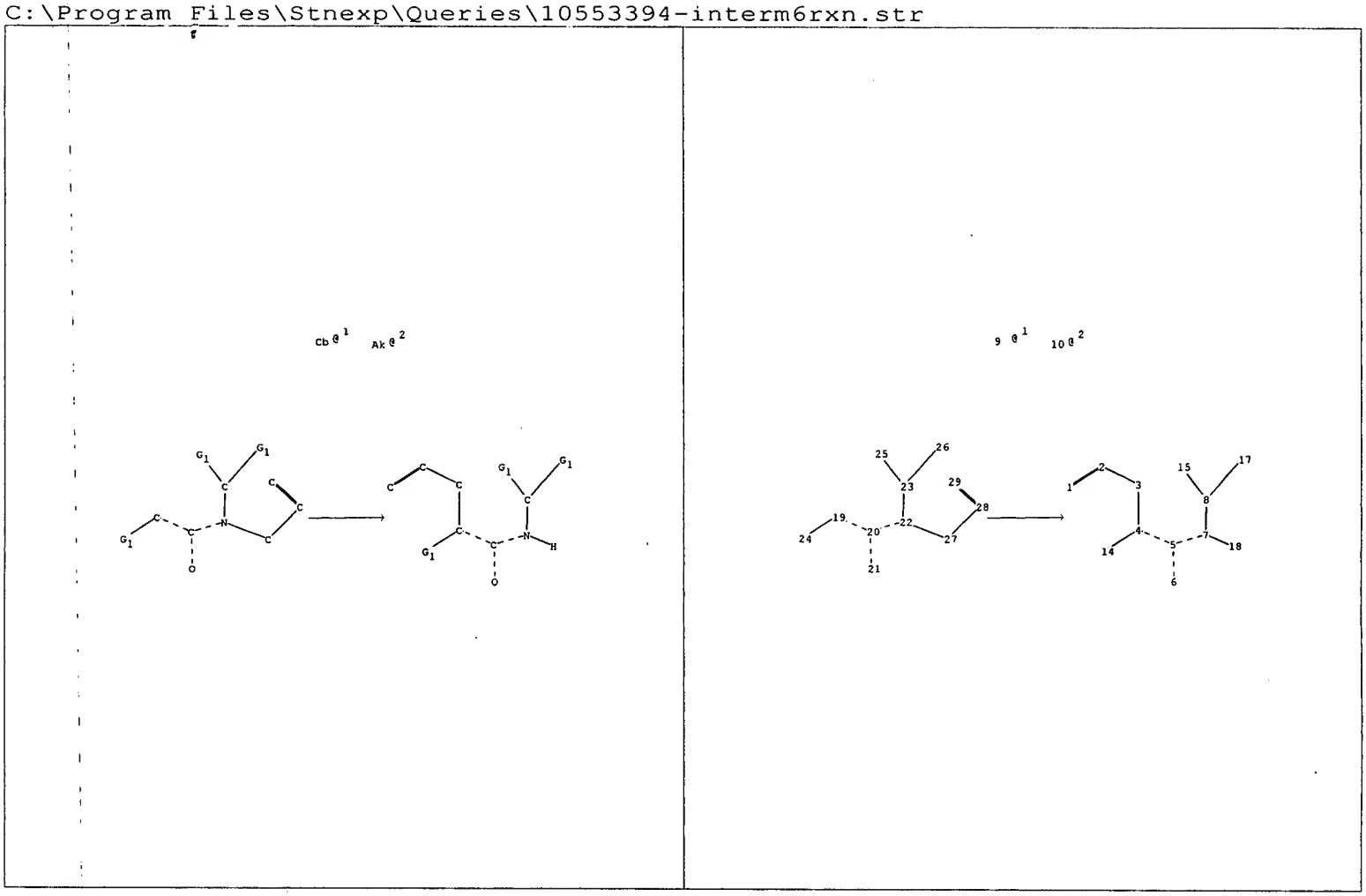
C:\Program Files\Stnexp\Queries\10553394-interm6rxn.str




```
chain nodes :
    1  2  3  4  5  6  7  8  9  10  14  15  17  18  19  20  21  22  23  24  25
    26  27  28  29
chain bonds :
    1-2  2-3  3-4  4-5  4-14  5-6  5-7  7-8  7-18  8-15  8-17  19-24  19-20
    20-21  20-22  22-23  22-27  23-25  23-26  27-28  28-29
exact/norm bonds :
    1-2  2-3  3-4  4-5  4-14  5-6  5-7  7-8  7-18  8-15  8-17  19-24  19-20
    20-21  20-22  22-23  22-27  23-25  23-26  27-28  28-29

G1:[*1],[*2]

Match level :
    1:CLASS  2:CLASS  3:CLASS  4:CLASS  5:CLASS  6:CLASS  7:CLASS  8:CLASS
    9:Atom  10:CLASS  14:CLASS  15:CLASS  17:CLASS  18:CLASS  19:CLASS
    20:CLASS  21:CLASS  22:CLASS  23:CLASS  24:CLASS  25:CLASS  26:CLASS
    27:CLASS  28:CLASS  29:CLASS
Generic attributes :
    9:
    Saturation              : Unsaturated
    10:
    Saturation              : Saturated

fragments assigned product role:
    containing 1
fragments assigned reactant/reagent role:
    containing 19
node mappings:
    7:22  8:23  3:27  2:28  1:29
```

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssptasjl1626

PASSWORD:
* * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'STNGUIDE' AT 07:16:40 ON 21 MAY 2007
FILE 'STNGUIDE' ENTERED AT 07:16:40 ON 21 MAY 2007

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.18	99.77

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.34

=> fil casreact

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.24	99.83

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.34

FILE 'CASREACT' ENTERED AT 07:17:13 ON 21 MAY 2007

FILE CONTENT:1840 - 19 May 2007 VOL 146 ISS 22

New CAS Information Use Policies, enter HELP USAGETERMS for details.

****
*
* CASREACT now has more than 12 million reactions *
*
****

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999)
provided by InfoChem, INPI data prior to 1986, and Biotransformations
database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance
identification.

=>
Uploading C:\Program Files\Stnexp\Queries\10553394-interm6rxn.str

L9 STRUCTURE UPLOADED

```
=> s l9
SAMPLE SEARCH INITIATED 07:17:35 FILE 'CASREACT'
SCREENING COMPLETE -     1381 REACTIONS TO VERIFY FROM      100 DOCUMENTS

100.0% DONE    1381 VERIFIED       0 HIT RXNS                        0 DOCS
SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS:     25393 TO    29847
PROJECTED ANSWERS:               0 TO        0

L10           0 SEA SSS SAM L9 (     0 REACTIONS)

=> s l9 sss full
FULL SEARCH INITIATED 07:17:48 FILE 'CASREACT'
SCREENING COMPLETE -    33987 REACTIONS TO VERIFY FROM     2032 DOCUMENTS

100.0% DONE   33987 VERIFIED       6 HIT RXNS                        4 DOCS
SEARCH TIME: 00.00.09

L11           4 SEA SSS FUL L9 (     6 REACTIONS)

=> d tot l11 all


L11  ANSWER 1 OF 4  CASREACT  COPYRIGHT 2007 ACS on STN
AN   140:27646  CASREACT
TI   Double diastereoselective [3,3]-sigmatropic aza-Claisen rearrangements
AU   Davies, Stephen G.; Garner, A. Christopher; Nicholson, Rebecca L.;
     Osborne, James; Savory, Edward D.; Smith, Andrew D.
CS   Dyson Perrins Laboratory, University of Oxford, Oxford, OX1 3QY, UK
SO   Chemical Communications (Cambridge, United Kingdom) (2003), (17),
     2134-2135
     CODEN: CHCOFS; ISSN: 1359-7345
PB   Royal Society of Chemistry
DT   Journal
LA   English
CC   25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
     Section cross-reference(s): 75
AB   Asym. [3,3]-sigmatropic aza-Claisen rearrangement of the
     (Z)-N-allyl-N,O-silylketene aminal of (3S,4E,αR)-1-benzyloxy-3-(N-
     propionyl-N-α-methylbenzylamino)hex-4-ene furnishes
     (2S,3R,4E,αR)-N-α-methylbenzyl-2,3-dimethyl-7-benzyloxyhept-4-
     enamide in >92% d.e.; rearrangement of the diastereomeric
     (3R,4E,αR)-(Z)-N,O-silylketene aminal proceeds with low
     diastereoselectivity.
ST   methylbenzyldimethylbenzyloxyheptenamide prepn double diastereoselective
     sigmatropic aza Claisen rearrangement
IT   Rearrangement
        ([3,3]-sigmatropic, stereoselective; preparation of
        methylbenzyldimethylbenzyloxyheptenamide via double diastereoselective
        [3,3]-sigmatropic aza-Claisen rearrangements)
IT   Claisen rearrangement
        (aza-, stereoselective; preparation of methylbenzyldimethylbenzyloxyheptenam
        ide via double diastereoselective [3,3]-sigmatropic aza-Claisen
        rearrangements)
IT   Crystal structure
     Molecular structure
        (of methylbenzyldimethylbenzyloxyheptenamide prepared via double
        diastereoselective [3,3]-sigmatropic aza-Claisen rearrangements)
IT   Asymmetric synthesis and induction
        (preparation of methylbenzyldimethylbenzyloxyheptenamide via double
```

diastereoselective [3,3]-sigmatropic aza-Claisen rearrangements)
IT Rearrangement
(stereoselective; preparation of methylbenzyldimethylbenzyloxyheptenamide via double diastereoselective [3,3]-sigmatropic aza-Claisen rearrangements)
IT 634599-72-7P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystal structure; preparation and crystal structure of methylbenzyldimethylbenzyloxyheptenamide from double diastereoselective [3,3]-sigmatropic aza-Claisen rearrangements)
IT 100-39-0, Benzyl bromide 81838-85-9 163234-78-4 185432-58-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of methylbenzyldimethylbenzyloxyheptenamide via double diastereoselective [3,3]-sigmatropic aza-Claisen rearrangements)
IT 257907-86-1P 257907-87-2P 257907-88-3P 634599-69-2P 634599-70-5P 634599-71-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of methylbenzyldimethylbenzyloxyheptenamide via double diastereoselective [3,3]-sigmatropic aza-Claisen rearrangements)
IT 634599-73-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of methylbenzyldimethylbenzyloxyheptenamide via double diastereoselective [3,3]-sigmatropic aza-Claisen rearrangements)
RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE

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(2) Enders, D; Tetrahedron: Asymmetry 1996, V7, P1847 CAPLUS
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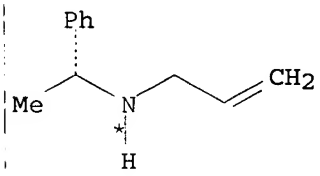
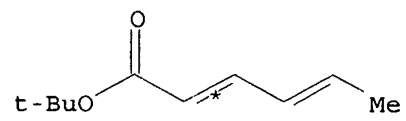
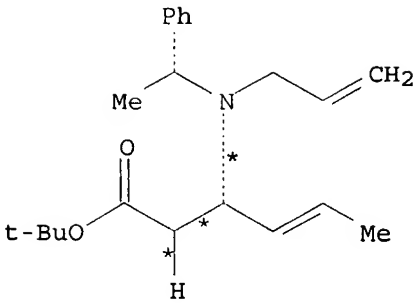
(18) Yamazaki, T; Tetrahedron Lett 1991, V32, P4267 CAPLUS
(19) Yoon, T; J Am Chem Soc 2001, V123, P2911 CAPLUS

RX(1) OF 16 A + B ===> C...





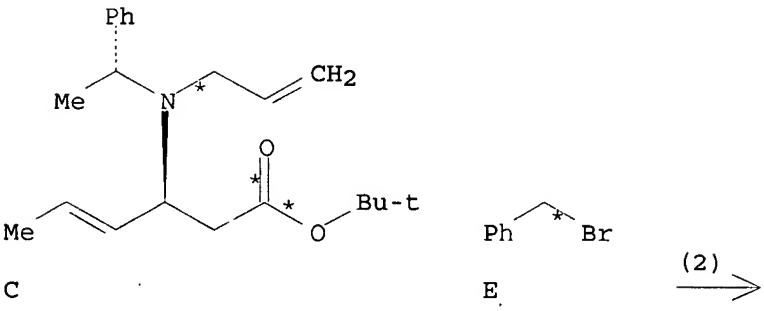
A B (1) ⟶



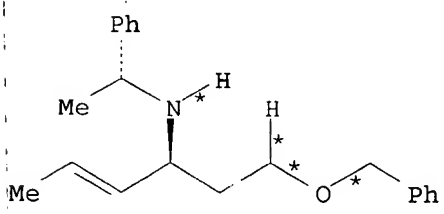
C
YIELD 85%

RX(1) RCT A 163234-78-4, B 81838-85-9
PRO C 257907-86-1
SOL 109-99-9 THF
CON -78 deg C
NTE stereoselective

RX(2) OF 16 ...C + E ===> F...



C E



F
YIELD 59%

RX(2) RCT C 257907-86-1

STAGE(1)
RGT G 16853-85-3 LiAlH4
SOL 109-99-9 THF
CON 0 deg C -> room temperature

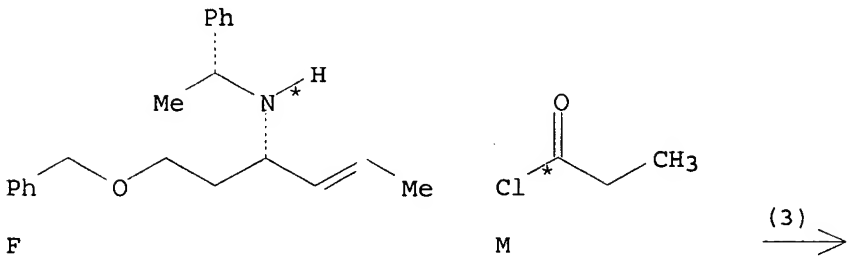
STAGE(2)

RCT E 100-39-0
RGT H 7646-69-7 NaH, I 33100-27-5 15-Crown-5

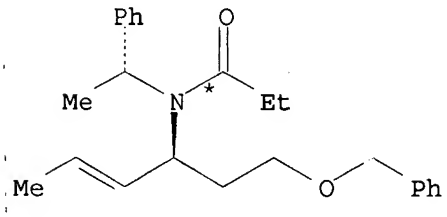
STAGE(3)
RGT J 14694-95-2 RhCl(PPh3)3
SOL 75-05-8 MeCN, 7732-18-5 Water

PRO F 634599-69-2
NTE stereoselective

RX(3) OF 16 ...F + M ===> N...



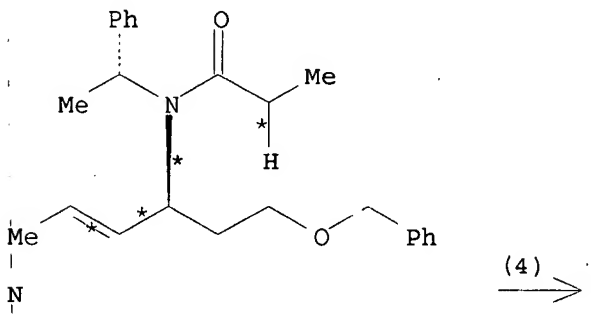
F M



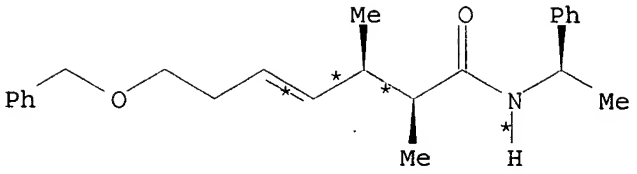
N
YIELD 99%

RX(3) RCT F 634599-69-2, M 79-03-8
RGT O 121-44-8 Et3N, P 1122-58-3 4-DMAP
PRO N 634599-70-5
SOL 75-09-2 CH2Cl2
CON room temperature

RX(4) OF 16 ...N ===> R



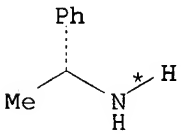
N

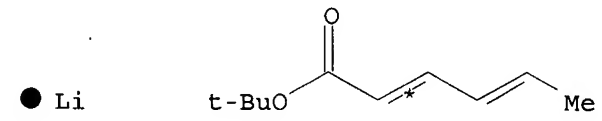


R
YIELD 90%

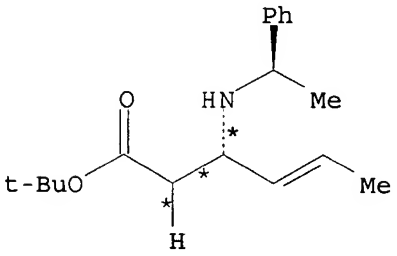
RX(4) RCT N 634599-70-5
RGT S 4039-32-1 (Me3Si)2N.Li, T 75-77-4 Me3SiCl
PRO R 634599-72-7
SOL 108-88-3 PhMe
CON reflux
NTE aza-Claisen rearrangement, stereoselective

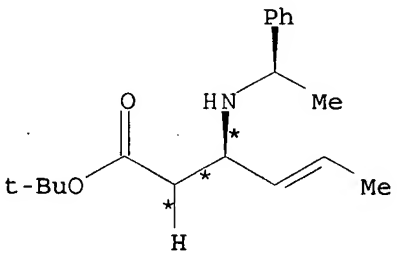
RX(5) OF 16 2 V + 2 B ===> W + X...





2 V 2 B (5) ⟶



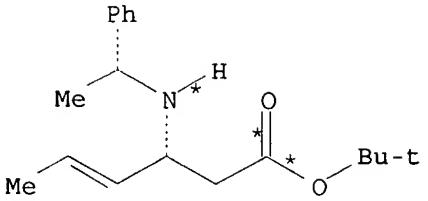


W
YIELD 25%

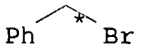
X
YIELD 15%

RX(5) RCT V 185432-58-0, B 81838-85-9
PRO W 257907-87-2, X 257907-88-3
SOL 109-99-9 THF
CON -78 deg C
NTE stereoselective

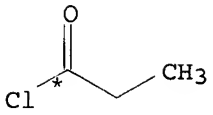
RX(6) OF 16 ...X + E + M ===> Y...



X

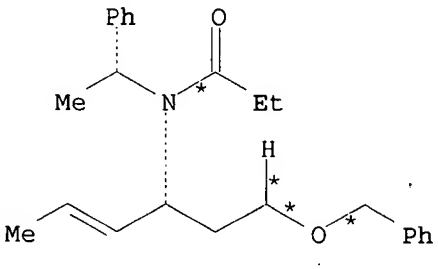


E



M

(6)



Y

RX(6) RCT X 257907-88-3

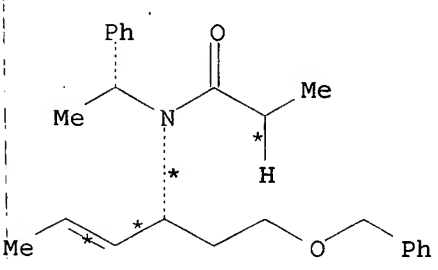
STAGE(1)
RGT G 16853-85-3 LiAlH4
SOL 109-99-9 THF
CON 0 deg C -> room temperature

STAGE(2)
RCT E 100-39-0
RGT H 7646-69-7 NaH, I 33100-27-5 15-Crown-5

STAGE(3)
RCT M 79-03-8
RGT O 121-44-8 Et3N, P 1122-58-3 4-DMAP
SOL 75-09-2 CH2Cl2
CON room temperature

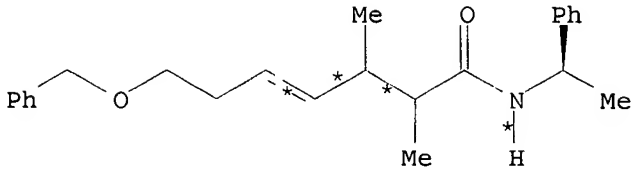
PRO Y 634599-71-6

RX(7) OF 16 ...Y ===> Z



Y

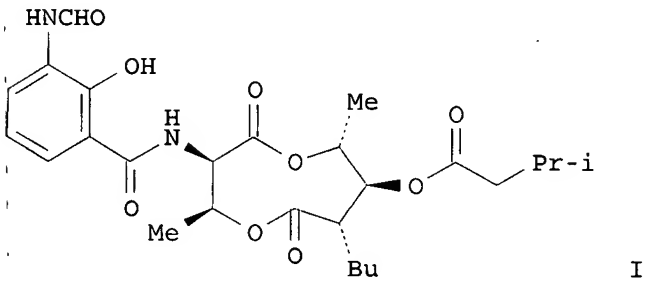
(7)



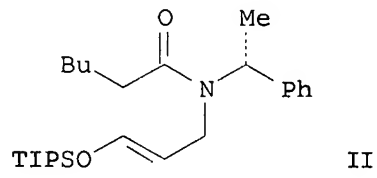
Z
YIELD 51%

RX(7) RCT Y 634599-71-6
RGT S 4039-32-1 (Me3Si)2N.Li, T 75-77-4 Me3SiCl
PRO Z 634599-73-8
SOL 108-88-3 PhMe
CON reflux
NTE aza-Claisen rearrangement, stereoselective, product obtained is inseparable mixt. of 3 of 8 possible diastereomers

L11 ANSWER 2 OF 4 CASREACT COPYRIGHT 2007 ACS on STN
AN 134:56500 CASREACT
TI A total synthesis of (-)-antimycin A3b
AU Tsunoda, Tetsuto; Nishii, Takeshi; Yoshizuka, Makoto; Yamasaki, Chise; Suzuki, Tomonori; Ito, Sho
CS Faculty of Pharmaceutical Sciences, Tokushima Bunri University, Tokushima, 770-8514, Japan
SO Tetrahedron Letters (2000), 41(40), 7667-7671
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier Science Ltd.
DT Journal
LA English
CC 26-6 (Biomolecules and Their Synthetic Analogs)
GI



I



II

AB (-)-Antimycin A3b (I), the antipode of natural antibiotic antimycin A3b, was synthesized utilizing the asym. aza-Claisen rearrangement of II.
ST antimycin A3b synthesis aza Claisen rearrangement

IT Claisen rearrangement
(aza-, asym.; total synthesis of (-)-antimycin A3b)
IT 312729-31-0P
RL: BYP (Byproduct); PREP (Preparation)
(total synthesis of (-)-antimycin A3b)
IT 107-02-8, Acrolein, reactions 142-61-0, Hexanoyl chloride 870-63-3, Prenyl bromide 1468-39-9, Isovaleric anhydride 2127-03-9, 2,2'-Dipyridyl disulfide 3886-69-9 312729-34-3 312729-40-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(total synthesis of (-)-antimycin A3b)
IT 312729-27-4P 312729-28-5P 312729-29-6P 312729-30-9P 312729-32-1P 312729-33-2P 312729-35-4P 312729-36-5P 312729-37-6P 312729-38-7P 312729-39-8P 312729-41-2P 312729-42-3P 312729-43-4P 313976-89-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(total synthesis of (-)-antimycin A3b)
IT 98587-10-1P 139066-86-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(total synthesis of (-)-antimycin A3b)
RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE

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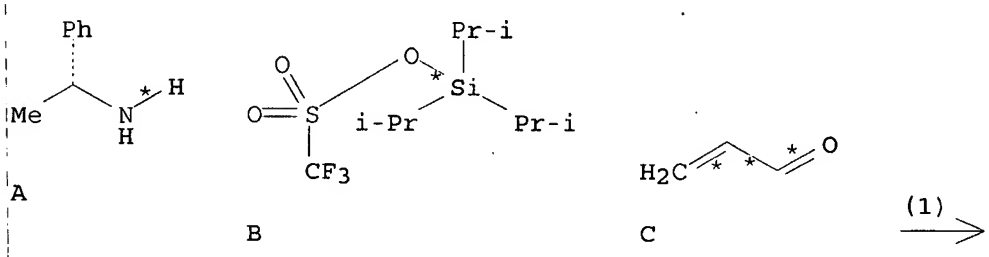
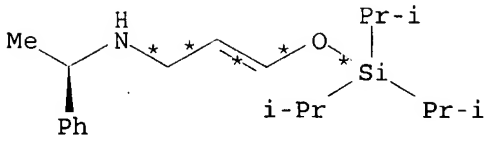
(19) Tsunoda, T; Chem Lett 1994, P543 CAPLUS
(20) Tsunoda, T; Tetrahedron Lett 1992, V33, P1651 CAPLUS
(21) Tsunoda, T; Tetrahedron Lett 1993, V34, P3297 CAPLUS
(22) Tsunoda, T; Tetrahedron Lett 1996, V37, P2463 CAPLUS
(23) Tsunoda, T; to be published
(24) Wasserman, H; J Am Chem Soc 1985, V107, P1423 CAPLUS
(25) Wasserman, H; Tetrahedron 1992, V48, P7059 CAPLUS
(26) Wikstrom, M; Biochim Biophys Acta 1972, V283, P403 CAPLUS

RX(1) OF 136 A + B + C ===> D...



A B C



D
YIELD 64%

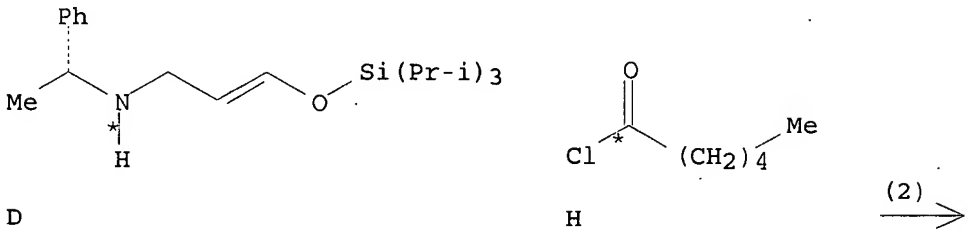
RX(1) RCT A 3886-69-9

STAGE(1)
RGT E 27607-77-8 Me3SiSO3CF3, F 6674-22-2 DBU
SOL 60-29-7 Et2O

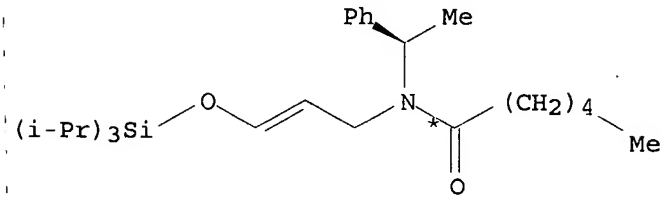
STAGE(2)
RCT B 80522-42-5, C 107-02-8
SOL 60-29-7 Et2O

PRO D 312729-27-4
NTE STEREOSELECTIVE

RX(2) OF 136 ...D + H ===> I...



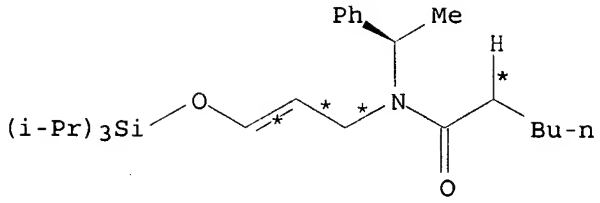
D H



I
YIELD 98%

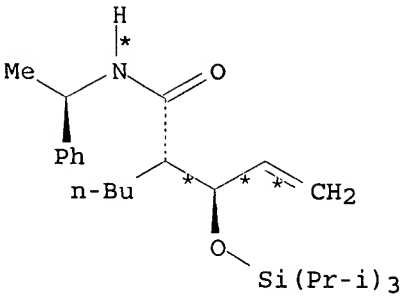
RX(2) RCT D 312729-27-4, H 142-61-0
RGT J 121-44-8 Et3N
PRO I 312729-28-5
SOL 75-09-2 CH2Cl2
NTE STEREOSELECTIVE

RX(3) OF 136 ...I ===> L...



I

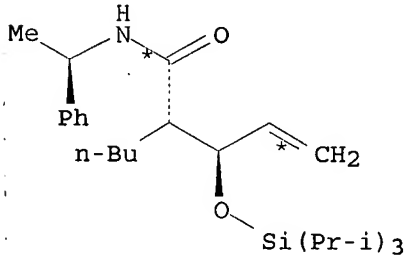
(3)



L
YIELD 78%

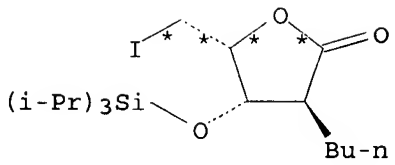
RX(3) RCT I 312729-28-5
RGT M 4039-32-1 (Me3Si)2N.Li
PRO L 312729-29-6
SOL 108-88-3 PhMe
NTE STEREOSELECTIVE

RX(4) OF 136 ...L ===> O...



L

(4)



O
YIELD 78%

RX(4) RCT L 312729-29-6
RGT P 7646-69-7 NaH, Q 100-23-2 Benzenamine, N,N-dimethyl-4-nitro-
PRO O 312729-30-9
SOL 68-12-2 DMF, 7732-18-5 Water
NTE STEREOSELECTIVE

RX(5) OF 136 ...O ===> T...

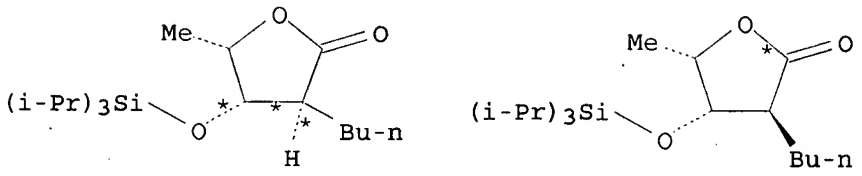
O

(5)

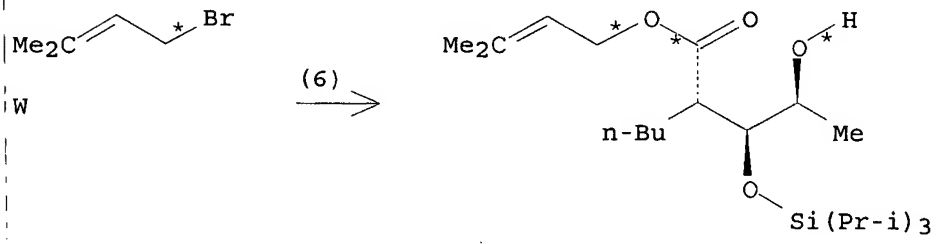
T
YIELD 91%

RX(5) RCT O 312729-30-9
RGT U 688-73-3 Bu3SnH
PRO T 312729-32-1
SOL 71-43-2 Benzene
NTE STEREOSELECTIVE

RX(6) OF 136 ...2 T + W ===> X + Y...



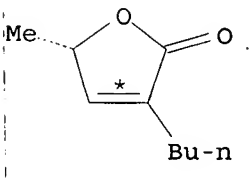
T T



W

(6)

X
YIELD 40%



Y
YIELD 40%

RX(6) RCT T 312729-32-1

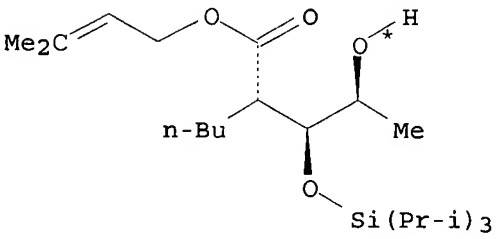
STAGE(1)
RGT Z 21351-79-1 CsOH

SOL 75-65-0 t-BuOH

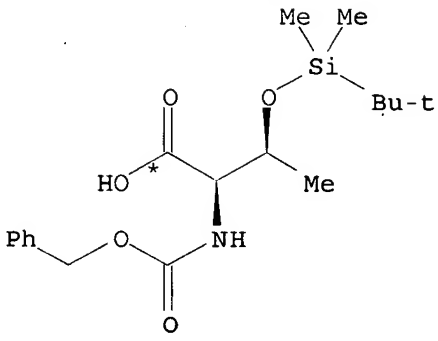
STAGE(2)
RCT W 870-63-3
RGT AA 110-86-1 Pyridine
SOL 60-29-7 Et2O

PRO X 312729-33-2, Y 98587-10-1
NTE STEREOSELECTIVE

RX(7) OF 136 ...X + AC ===> AD...

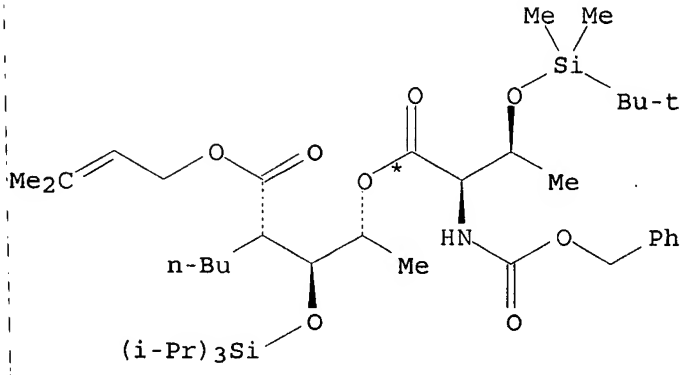


X



AC

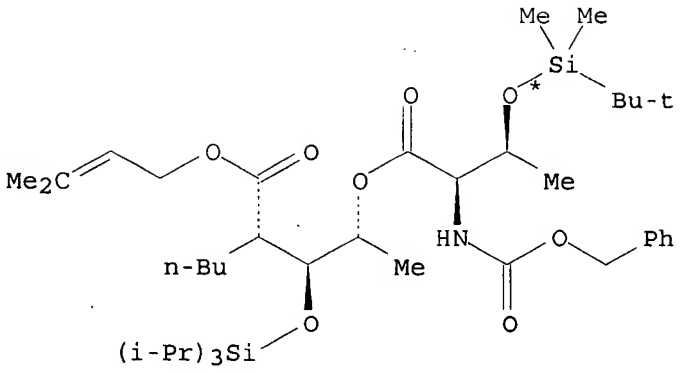
(7)



AD
YIELD 100%

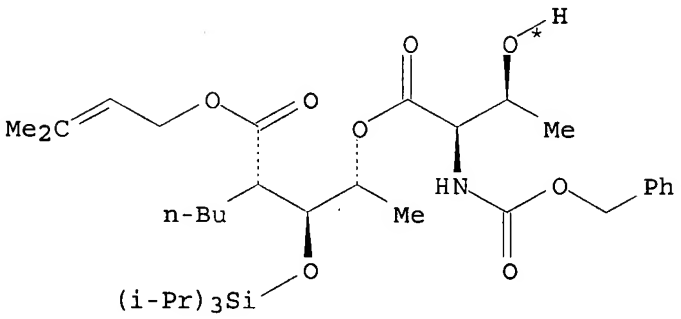
RX(7) RCT X 312729-33-2, AC 312729-34-3
RGT AE 1972-28-7 EtO2CN:NCO2Et, AF 603-35-0 PPh3
PRO AD 312729-35-4
SOL 71-43-2 Benzene
NTE STEREOSELECTIVE

RX(8) OF 136 ...AD ===> AG...



AD

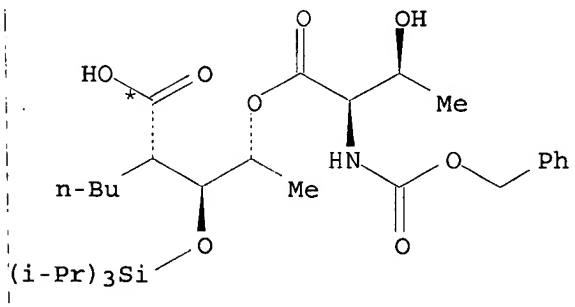
(8)



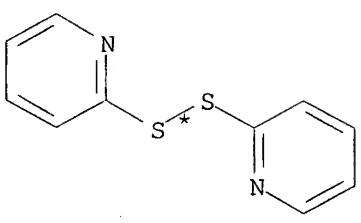
AG
YIELD 95%

RX(8) RCT AD 312729-35-4
RGT AH 7647-01-0 HCl
PRO AG 312729-43-4
SOL 64-17-5 EtOH
NTE STEREOSELECTIVE

RX(9) OF 136 ...AJ + AK ===> AL...

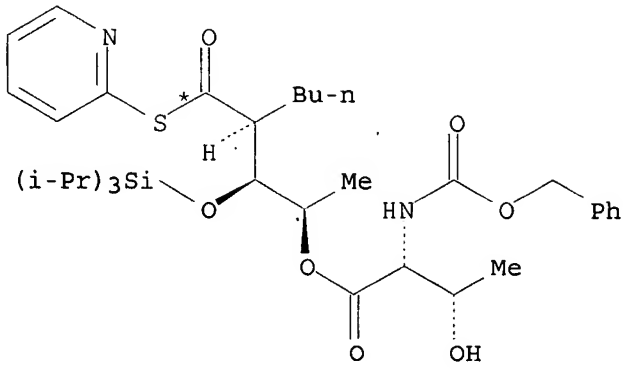


AJ



AK

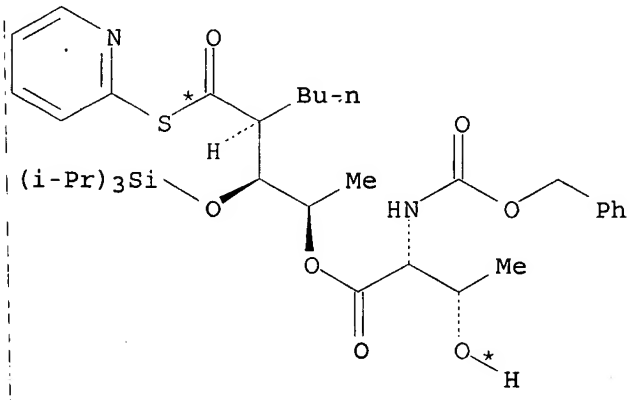
(9)



AL
YIELD 99%

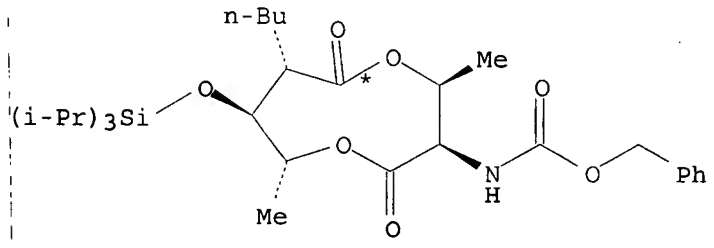
RX(9) RCT AJ 312729-36-5, AK 2127-03-9
RGT AF 603-35-0 PPh3
PRO AL 312729-37-6
SOL 71-43-2 Benzene
NTE STEREOSELECTIVE

RX(10) OF 136 ...AL ===> AM...



AL

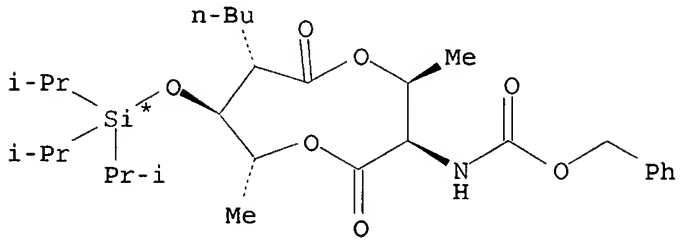
(10)



AM
YIELD 82%

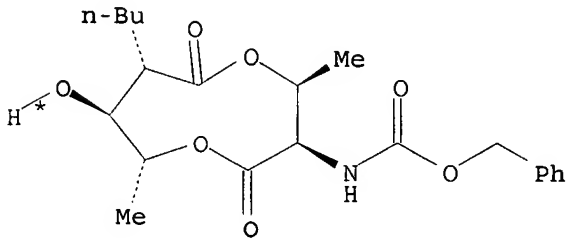
RX(10) RCT AL 312729-37-6
        RGT AN 7783-93-9 AgClO4
        PRO AM 312729-38-7
        SOL 71-43-2 Benzene
        NTE STEREOSELECTIVE

RX(11) OF 136 ...AM ===> AO...



AM

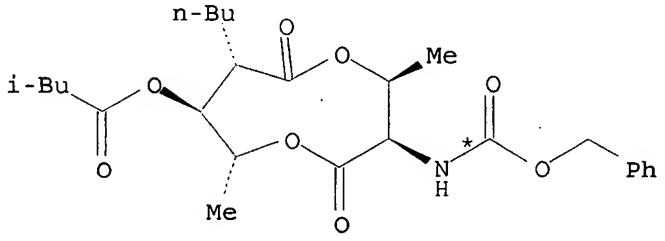
(11)



AO
YIELD 85%

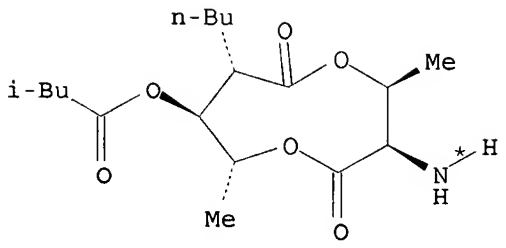
RX(11) RCT AM 312729-38-7
        RGT AP 429-41-4 Bu4N.F
        PRO AO 312729-42-3
        SOL 109-99-9 THF
        NTE STEREOSELECTIVE

RX(12) OF 136 ...AR ===> AS...



AR

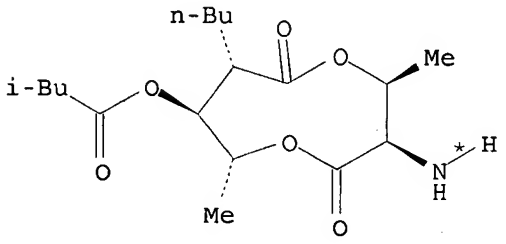
(12)



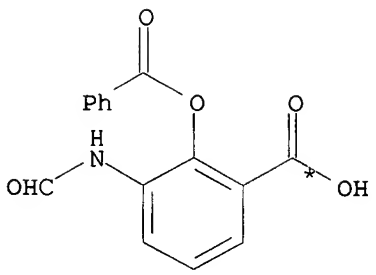
AS
YIELD 67%

RX(12) RCT AR 313976-89-5
RGT AT 1333-74-0 H2
PRO AS 312729-39-8
CAT 7440-05-3 Pd
SOL 141-78-6 AcOEt
NTE STEREOSELECTIVE

RX(13) OF 136 ...AS + AW ===> AX...

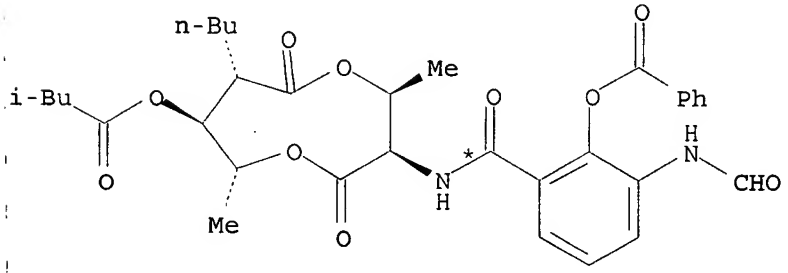


AS



AW

(13)

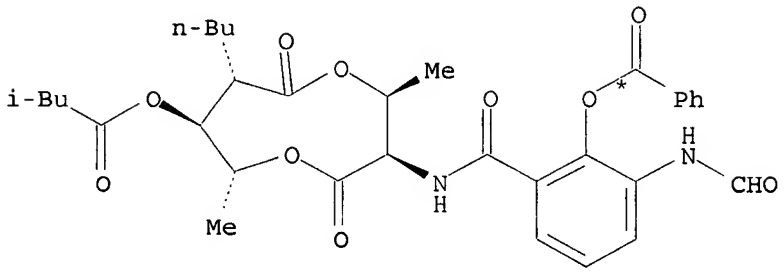


AX
YIELD 95%

RX(13) RCT AS 312729-39-8, AW 312729-40-1
RGT AY 2592-95-2 1-Benzotriazolol, AZ 109-02-4 N-Methylmorpholine,
BA 25952-53-8 EDAP
PRO AX 312729-41-2

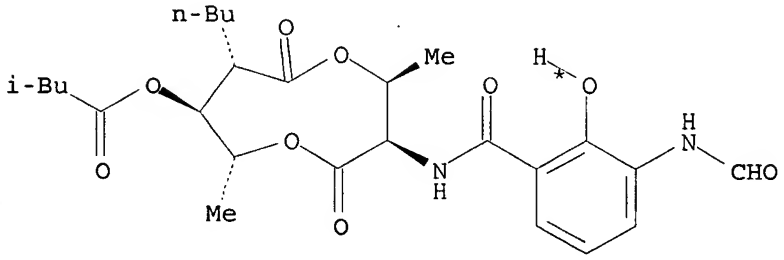
SOL 68-12-2 DMF
NTE STEREOSELECTIVE

RX(14) OF 136 ...AX ===> BB



AX

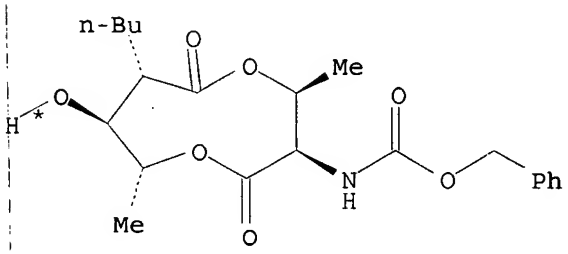
(14)



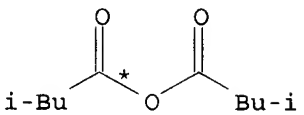
BB
YIELD 89%

RX(14) RCT AX 312729-41-2
RGT AT 1333-74-0 H2
PRO BB 139066-86-7
CAT 7440-05-3 Pd
SOL 141-78-6 AcOEt
NTE STEREOSELECTIVE

RX(15) OF 136 ...AO + BC ===> AR...

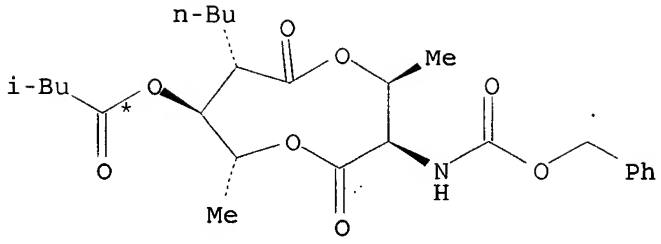


AO



BC

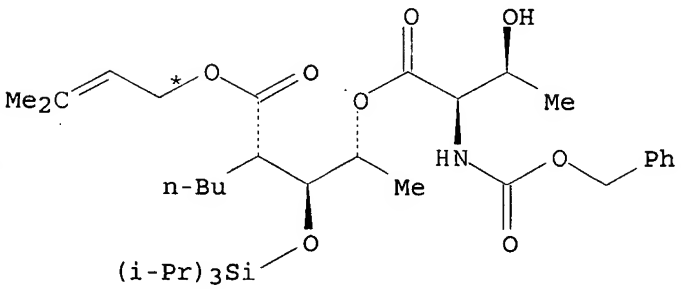
(15)



AR
YIELD 53%

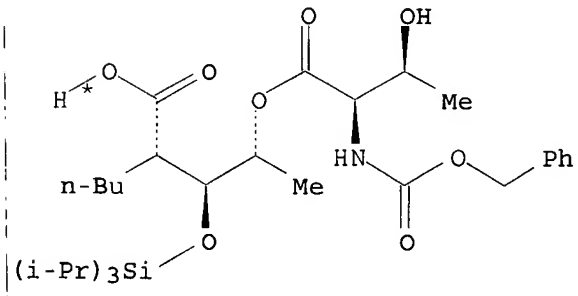
RX(15) RCT AO 312729-42-3, BC 1468-39-9
PRO AR 313976-89-5
SOL 110-86-1 Pyridine
NTE STEREOSELECTIVE

RX(16) OF 136 ...AG ===> AJ...



AG

(16)

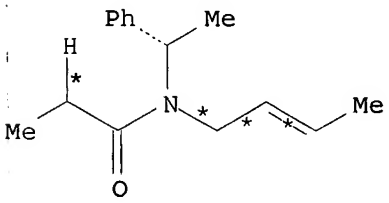


AJ
YIELD 85%

RX(16) RCT AG 312729-43-4
RGT BD 3375-31-3 Pd(OAc)2, AF 603-35-0 PPh3, J 121-44-8 Et3N, BE 64-18-6 HCO2H
PRO AJ 312729-36-5
SOL 123-91-1 Dioxane
NTE STEREOSELECTIVE

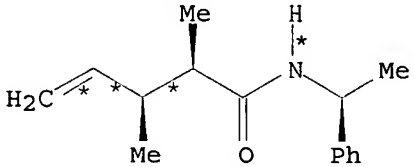
L11 ANSWER 3 OF 4 CASREACT COPYRIGHT 2007 ACS on STN
AN 116:255275 CASREACT
TI Asymmetric induction in aza-Claisen rearrangement of carboxamide enolates. Effect of chiral auxiliary on nitrogen
AU Tsunoda, Tetsuto; Sakai, Mika; Sasaki, Osamu; Sako, Yoshie; Hondo, Yuka; Ito, Sho
CS Fac. Pharm. Sci., Tokushima Bunri Univ., Tokushima, 770, Japan
SO Tetrahedron Letters (1992), 33(12), 1651-4
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
CC 25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
AB Aza-Claisen rearrangement of enolates of N-alkyl-N-(2E)-butenylpropanamides with chiral alkyl groups proceeded with high relative asym. induction as well as excellent internal asym. induction to give optically active N-alkyl-syn-2,3-dimethylpent-4-enamides.
ST asym aza Claisen rearrangement amide enolate
IT Asymmetric synthesis and induction
(in aza-Claisen rearrangement of carboxamide enolates)
IT Claisen rearrangement
(aza-, of carboxamide enolates)
IT Amides, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(enolates, aza-Claisen rearrangement of)
IT 130942-13-1 141423-08-7 141423-09-8 141423-10-1 141423-11-2 141423-12-3 141447-14-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. aza-Claisen rearrangement of)
IT 130942-15-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acylation of)
IT 141447-13-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
IT 141505-90-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and ozonolysis of)
IT 5866-39-7P 130983-06-1P 141423-02-1P 141423-03-2P 141423-04-3P 141423-05-4P 141423-06-5P 141423-07-6P 141505-84-2P 141505-85-3P 141505-86-4P 141505-87-5P 141505-88-6P 141505-89-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RX(1) OF 2 2 A ===> B + C

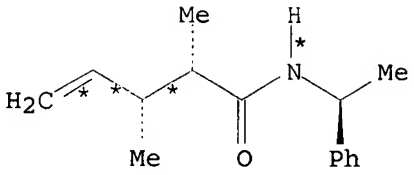


2 A

(1)



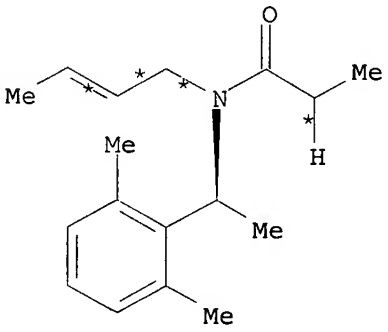
B
YIELD 79%(77)



C
YIELD 79%(22)

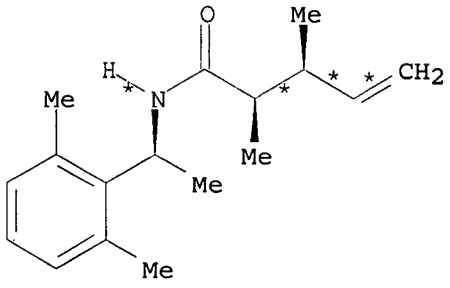
RX(1) RCT A 130942-13-1
RGT D 4111-54-0 LiN(Pr-i)2
PRO B 130942-15-3, C 130983-06-1
SOL 109-99-9 THF

RX(2) OF 2 2 F ===> G + H

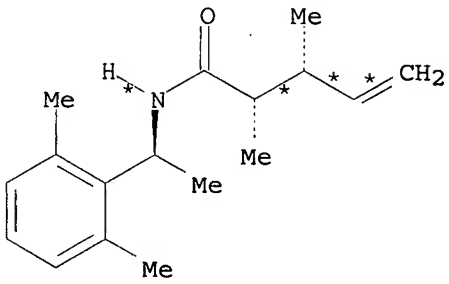


2 F

(2) ⟶



G
YIELD 90%(87)

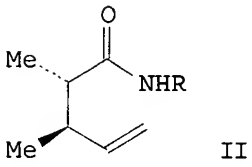


H
YIELD 90%(12)

RX(2) RCT F 141423-09-8
RGT I 4039-32-1 (Me3Si)2N.Li
PRO G 141423-03-2, H 141505-85-3
SOL 108-88-3 PhMe

L11 ANSWER 4 OF 4 CASREACT COPYRIGHT 2007 ACS on STN
AN 114:5978 CASREACT
TI A few new methods for asymmetric synthesis
AU Ito, Sho; Tsunoda, Tetsuto

CS Fac. Pharm. Sci., Tokushima Bunri Univ., Tokushima, 770, Japan
SO Pure and Applied Chemistry (1990), 62(7), 1405-8
CODEN: PACHAS; ISSN: 0033-4545
DT Journal
LA English
CC 25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 23
GI



II

AB Aza-Claisen rearrangement of (E)-EtCONRCH2CH:CHMe (I; R = Bu) was found to proceed smoothly at .apprx.135° in the presence of LDA to furnish II (R = Bu) in .apprx.94% yield and >99% diastereomeric excess (d.e.). The reaction of I (R = CHMePh) gave II (same R) in 83% d.e. An efficient and generally-applicable two-step procedure for the hydrolysis of N-monosubstituted amides was also developed and the corresponding carboxylic acids were obtained in good yields without any epimerization at the α-position of the acyl group. The amines used for the chiral induction can be recovered in 71% yield.
ST stereoselective aza Claisen rearrangement amide; hydrolysis monosubstituted amide
IT Amides, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(aza-Claisen rearrangement and hydrolysis of)
IT Stereochemistry
(of aza-Claisen rearrangement of propanamides)
IT Hydrolysis
(of monosubstituted amides)
IT Claisen rearrangement
(aza-, stereoselective, of propanamides)
IT 58908-50-2, Acetoxypivaloyl chloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(agent, for hydrolysis of monosubstituted amides)
IT 72592-55-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkylation by, of butylpropanamide)
IT 29576-14-5, E-Crotyl bromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkylation by, of propanamides)
IT 13022-17-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkylation of, with crotyl bromide)
IT 2955-67-1, N-Butylpropanamide
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkylation of, with crotyl bromide and tosylate)
IT 2782-40-3 10264-28-5 35665-26-0 61765-19-3 128037-34-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(amide hydrolysis of)
IT 2627-86-3P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, during hydrolysis of carbamate)
IT 128037-40-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrolysis of)
IT 128013-58-1P 128013-59-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and amide hydrolysis of)

IT 130942-13-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and aza-Claisen rearrangement of)

IT 128013-56-9P 128013-57-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and aza-Claisen rearrangement of, stereoselective)

IT 130942-19-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion of, to carbamate)

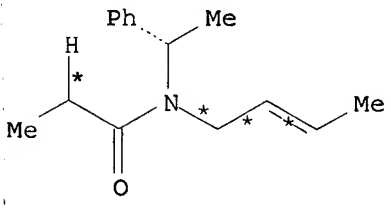
IT 33290-12-9P 128037-35-4P 128037-36-5P 128037-37-6P 128037-38-7P 130942-16-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

IT 130942-15-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and sequential ozonolysis and cyclization of, dimethylsuccinic acid from)

IT 5866-39-7P, (+)-2,3-Dimethylsuccinic acid 27069-03-0P 128037-41-2P 130942-12-0P 130942-14-2P 130942-17-5P 130942-18-6P 130983-06-1P 130983-07-2P 130983-08-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

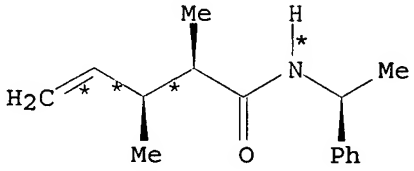
IT 65-85-0P, Benzoic acid, preparation 98-89-5P, Cyclohexanecarboxylic acid 142-62-1P, Hexanoic acid, preparation 58367-53-6P 58367-54-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by amide hydrolysis)

RX(1) OF 4 2 A ===> B + C

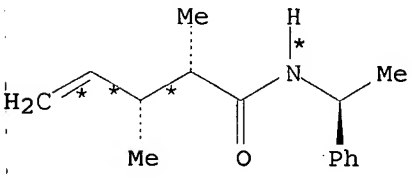


2 A

(1)



B
YIELD 85%(92)

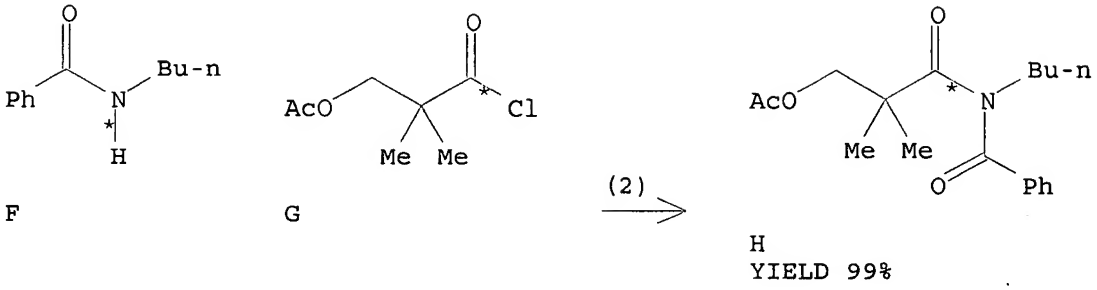


C
YIELD 85%(8)

RX(1) RCT A 130942-13-1
RGT D 4111-54-0 LiN(Pr-i)2
PRO B 130942-15-3, C 130983-06-1

SOL 108-88-3 PhMe

RX(2) OF 4 F + G ===> H...

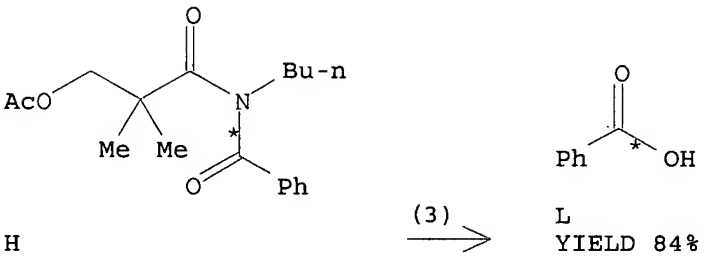


F G H

YIELD 99%

RX(2) RCT F 2782-40-3, G 58908-50-2
RGT I 121-44-8 Et3N, J 1122-58-3 4-DMAP
PRO H 128037-38-7
SOL 75-09-2 CH2Cl2

RX(3) OF 4 ...H ===> L



H L

YIELD 84%

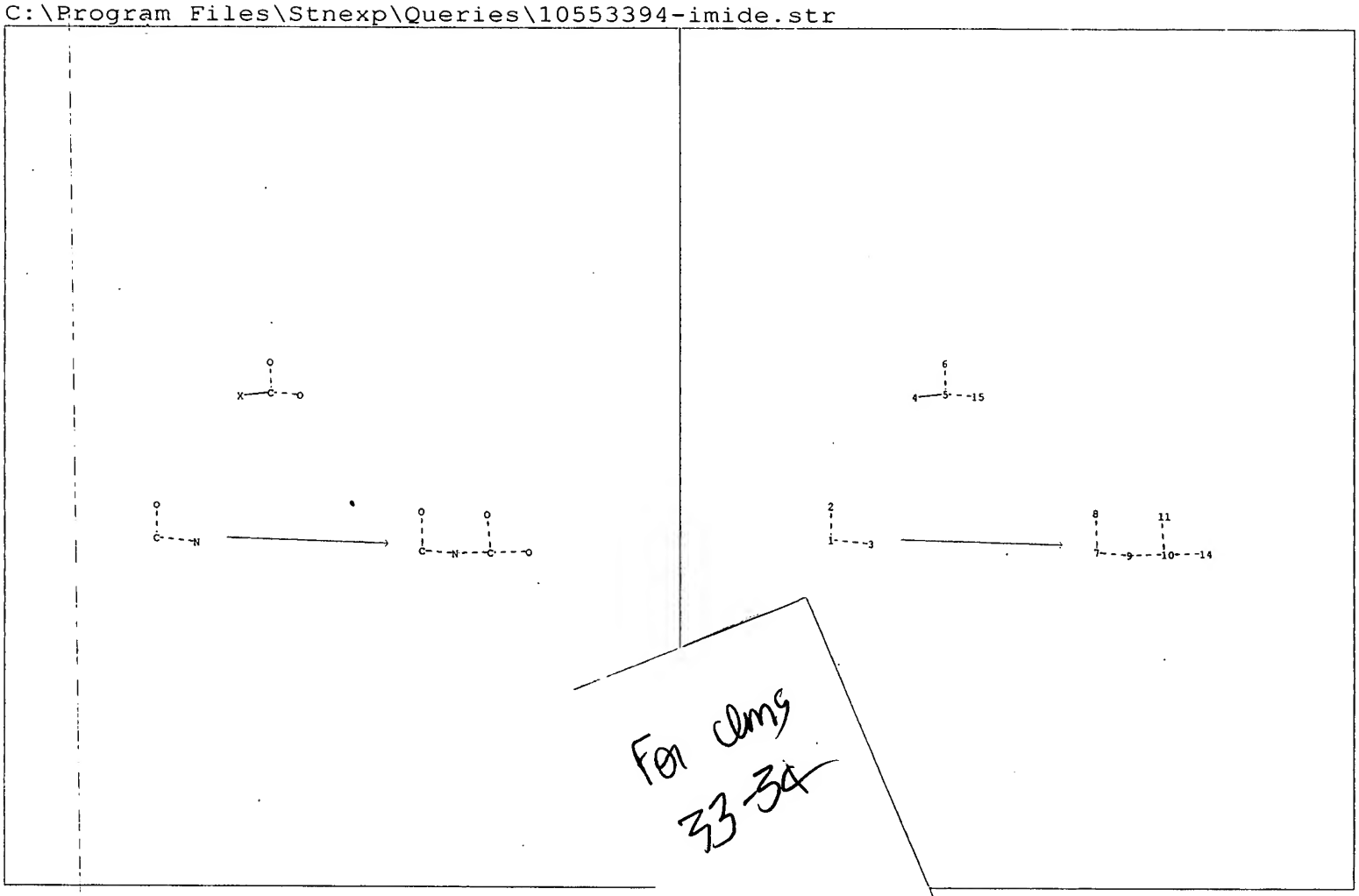
RX(3) RCT H 128037-38-7
RGT M 1310-65-2 LiOH
PRO L 65-85-0
SOL 109-99-9 THF

=> log hold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	147.62	247.45
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.92	-5.26

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 07:19:40 ON 21 MAY 2007

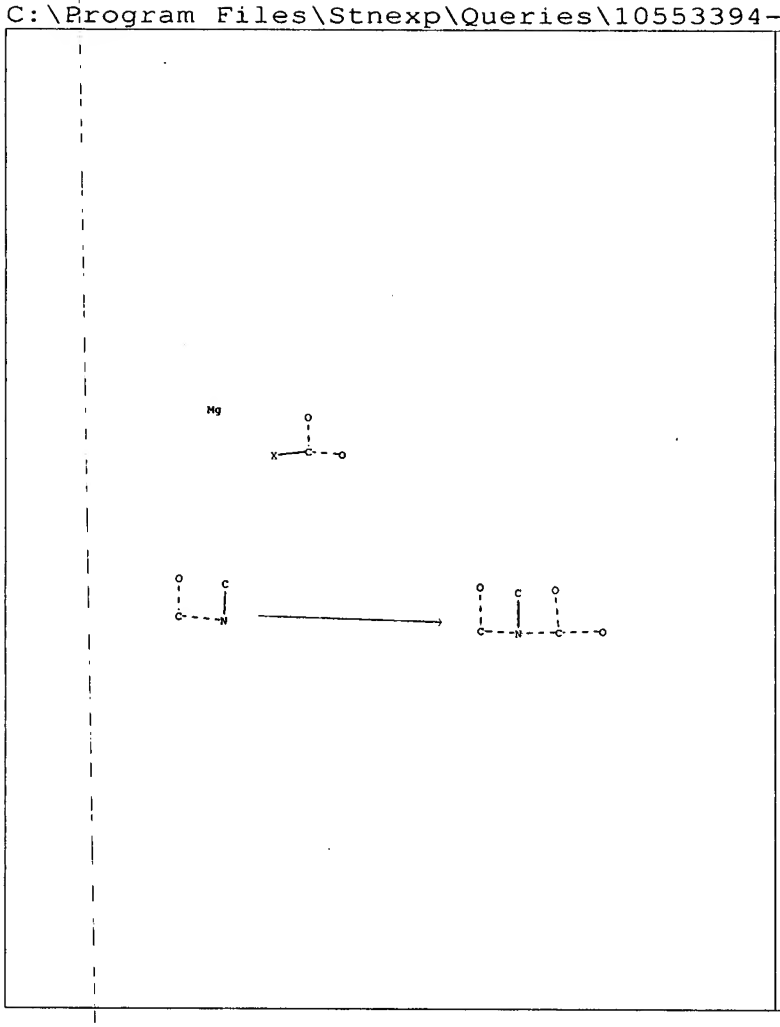
C:\Program Files\Stnexp\Queries\10553394-imide.str

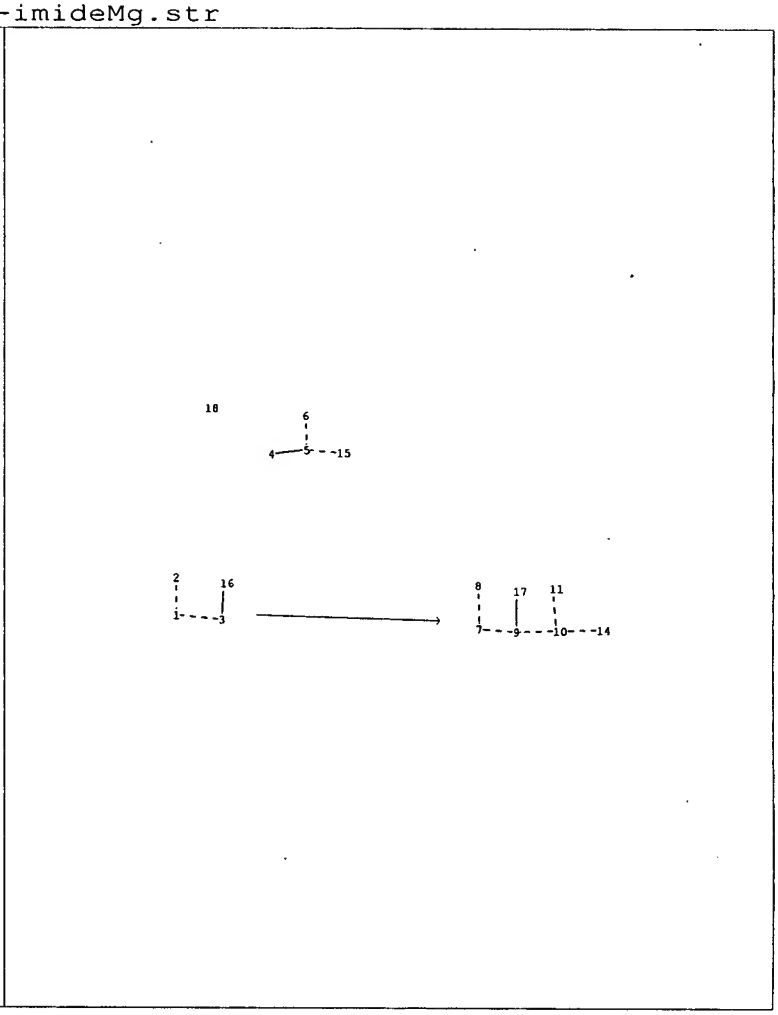



```
chain nodes :
    1  2  3  4  5  6  7  8  9  10  11  14
chain bonds :
    1-2  1-3  4-5  5-6  5-15  7-8  7-9  9-10  10-11  10-14
exact/norm bonds :
    1-2  1-3  4-5  5-6  5-15  7-8  7-9  9-10  10-11  10-14

Match level :
    1:CLASS  2:CLASS  3:CLASS  4:CLASS  5:CLASS  6:CLASS  7:CLASS  8:CLASS
    9:CLASS  10:CLASS  11:CLASS  14:CLASS  15:CLASS
fragments assigned product role:
    containing 7
fragments assigned reactant/reagent role:
    containing 1
    containing 4
node mappings:
    1:7  2:8  3:9  5:10  6:11  14:15  14:15
```

C:\Program Files\Stnexp\Queries\10553394-imideMg.str

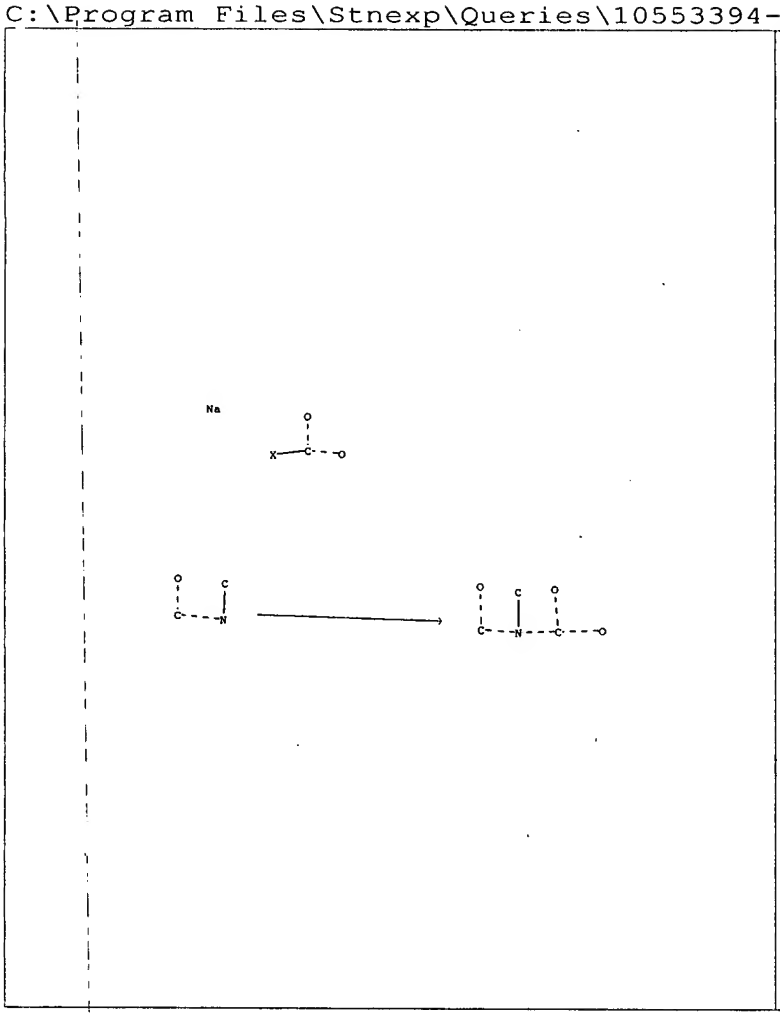


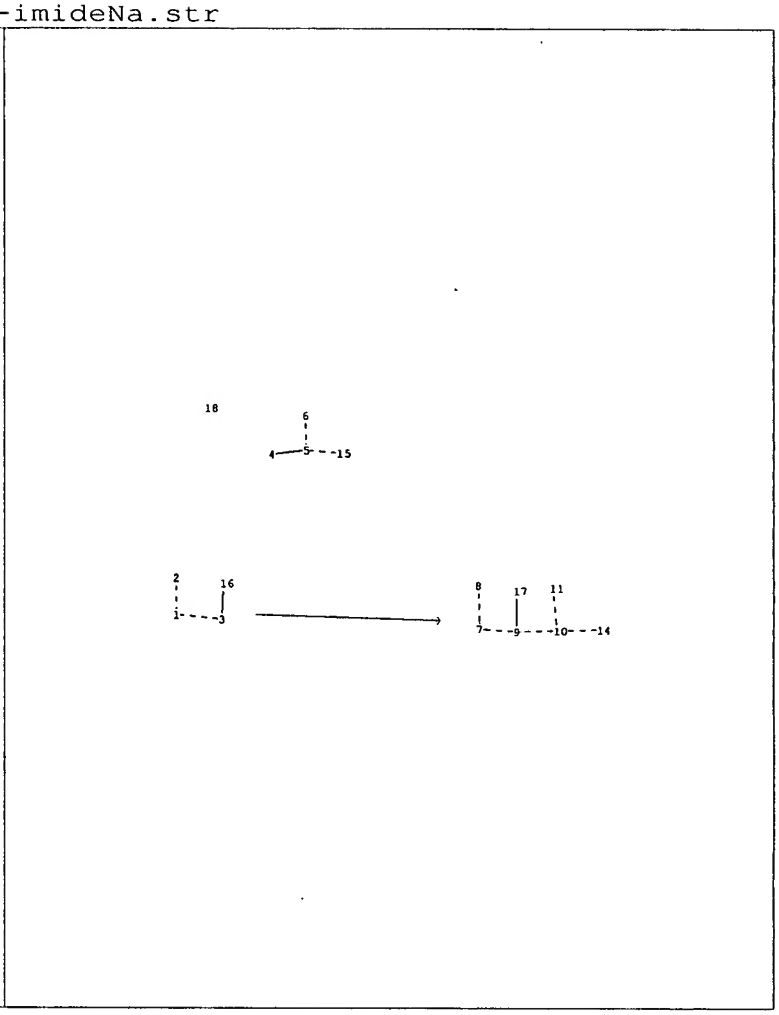


chain nodes :
1 2 3 4 5 6 7 8 9 10 11 14 15 16 17 18
chain bonds :
1-2 1-3 3-16 4-5 5-6 5-15 7-8 7-9 9-10 9-17 10-11 10-14
exact/norm bonds :
1-2 1-3 3-16 4-5 5-6 5-15 7-8 7-9 9-10 9-17 10-11 10-14

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS
9:CLASS 10:CLASS 11:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS
18:CLASS
fragments assigned product role:
containing 7
fragments assigned reactant/reagent role:
containing 1
containing 4
containing 18
node mappings:
1:7 2:8 3:9 5:10 6:11 14:15

C:\Program Files\Stnexp\Queries\10553394-imideNa.str





chain nodes :
1 2 3 4 5 6 7 8 9 10 11 14 15 16 17 18
chain bonds :
1-2 1-3 3-16 4-5 5-6 5-15 7-8 7-9 9-10 9-17 10-11 10-14
exact/norm bonds :
1-2 1-3 3-16 4-5 5-6 5-15 7-8 7-9 9-10 9-17 10-11 10-14

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS
9:CLASS 10:CLASS 11:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS
18:CLASS
fragments assigned product role:
containing 7
fragments assigned reactant/reagent role:
containing 1
containing 4
containing 18
node mappings:
1:7 2:8 3:9 5:10 6:11 14:15 14:15

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssptasjl1626

PASSWORD:
* * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'CASREACT' AT 07:59:47 ON 21 MAY 2007
FILE 'CASREACT' ENTERED AT 07:59:47 ON 21 MAY 2007
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	147.62	247.45

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.92	-5.26

=> fil casreact

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	147.62	247.45

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.92	-5.26

FILE 'CASREACT' ENTERED AT 07:59:56 ON 21 MAY 2007
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FILE CONTENT:1840 - 19 May 2007 VOL 146 ISS 22

New CAS Information Use Policies, enter HELP USAGETERMS for details.

****
*
* CASREACT now has more than 12 million reactions *
*
****

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>
Uploading C:\Program Files\Stnexp\Queries\10553394-imide.str

L12 STRUCTURE UPLOADED

```
=> s l12
SAMPLE SEARCH INITIATED 08:00:14 FILE 'CASREACT'
SCREENING COMPLETE -       35 REACTIONS TO VERIFY FROM        9 DOCUMENTS

100.0% DONE      35 VERIFIED      11 HIT RXNS                      3 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS:        346 TO     1054
PROJECTED ANSWERS:                3 TO      163

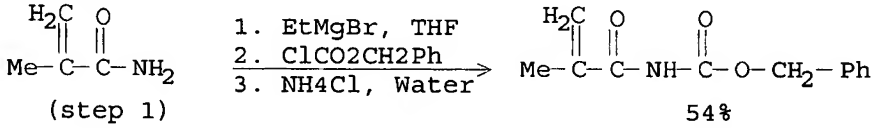
L13           3 SEA SSS SAM L12 (     11 REACTIONS)

=> d scan

L13  3 ANSWERS   CASREACT  COPYRIGHT 2007 ACS on STN

TI   Amine-Salt-Controlled, Catalytic Asymmetric Conjugate Addition of Various
     Amines and Asymmetric Protonation

RX(20) OF 27
```

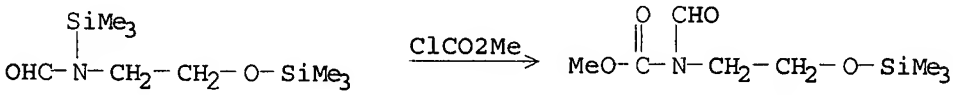



```
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):2

L13  3 ANSWERS   CASREACT  COPYRIGHT 2007 ACS on STN

TI   Synthesis of carbofunctional organosilicon compounds.  Silicon-containing
     amides and formamides

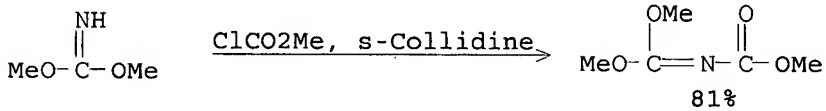
RX(18) OF 41
```




```
L13  3 ANSWERS   CASREACT  COPYRIGHT 2007 ACS on STN

TI   1,1,3,3-Tetraalkoxy-2-azaallylium salts:  synthesis and stereochemical
     properties

RX(3) OF 6
```




```
ALL ANSWERS HAVE BEEN SCANNED

=> fil stng
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                               0.45     247.90

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)    SINCE FILE      TOTAL
```

```
                                                        ENTRY    SESSION
CA SUBSCRIBER PRICE                                      0.00      -5.26

FILE 'STNGUIDE' ENTERED AT 08:00:29 ON 21 MAY 2007
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AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: May 18, 2007 (20070518/UP).

=> fil casreact
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                        ENTRY    SESSION
FULL ESTIMATED COST                                      0.24     248.14

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                        ENTRY    SESSION
CA SUBSCRIBER PRICE                                      0.00      -5.26

FILE 'CASREACT' ENTERED AT 08:03:10 ON 21 MAY 2007
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FILE CONTENT:1840 - 19 May 2007 VOL 146 ISS 22

New CAS Information Use Policies, enter HELP USAGETERMS for details.

*************************************************************
*                                                           *
*     CASREACT now has more than 12 million reactions       *
*                                                           *
*************************************************************

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999)
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This file contains CAS Registry Numbers for easy and accurate substance
identification.

=>
Uploading C:\Program Files\Stnexp\Queries\10553394-imide2.str

L14     STRUCTURE UPLOADED

=> s l14
SAMPLE SEARCH INITIATED 08:03:29 FILE 'CASREACT'
SCREENING COMPLETE -       15 REACTIONS TO VERIFY FROM        2 DOCUMENTS

100.0% DONE      15 VERIFIED       7 HIT RXNS                      1 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS:        68 TO      532
PROJECTED ANSWERS:               1 TO       79

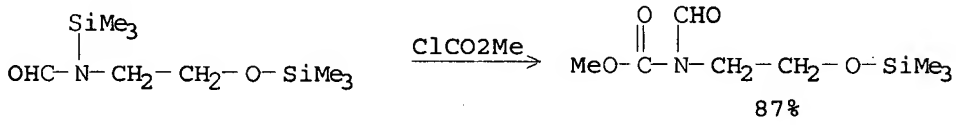
L15           1 SEA SSS SAM L14 (     7 REACTIONS)
```

```
=> d scan

L15  1 ANSWERS   CASREACT  COPYRIGHT 2007 ACS on STN

TI   Synthesis of carbofunctional organosilicon compounds.  Silicon-containing
     amides and formamides

RX(18) OF 41
```




```
ALL ANSWERS HAVE BEEN SCANNED


=> s l12 sss full
FULL SEARCH INITIATED 08:04:05 FILE 'CASREACT'
SCREENING COMPLETE -      2122 REACTIONS TO VERIFY FROM      247 DOCUMENTS

100.0% DONE    2122 VERIFIED     799 HIT RXNS (     85 INCOMP)      106 DOCS
SEARCH TIME: 00.00.02

L16         106 SEA SSS FUL L12 (    799 REACTIONS)

=> sav tem 3pr553394/a l16
3PR553394/A IS NOT A VALID SAVED NAME
Enter the name you wish to use for the saved query,
answer set, or L-number list.  The name must:
  1. Begin with a letter,
  2. Have 1-12 characters,
  3. Contain only letters (A-Z) and numbers (0-9),
  4. End with /Q for a query (search profile,
     structure, or screen set), /A for an answer
     set, or /L for an L-number list.
  5. Not already be in use as a saved name,
  6. Not be END, SAV, SAVE, SAVED
  7. Not have the form of an L-number (Lnnn).
ENTER NAME OR (END):imi553394/a

=> act imi553394/a
L17             STR
L18         106 SEA FILE=CASREACT SSS FUL L17 (    799 REACTIONS)

=> s l14 sub=l18 sss full
FULL SUBSET SEARCH INITIATED 08:05:56 FILE 'CASREACT'
SCREENING COMPLETE -       348 REACTIONS TO VERIFY FROM       61 DOCUMENTS

100.0% DONE     348 VERIFIED     161 HIT RXNS                     37 DOCS
SEARCH TIME: 00.00.01

L19          37 SEA SUB=L18 SSS FUL L14 (    161 REACTIONS)

=> fil stng
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                             130.05     378.19

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)    SINCE FILE      TOTAL
                                                 ENTRY    SESSION
CA SUBSCRIBER PRICE                               0.00      -5.26
```

```
FILE 'STNGUIDE' ENTERED AT 08:06:08 ON 21 MAY 2007
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FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: May 18, 2007 (20070518/UP).

=> fil casreact
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.24     378.43

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                         ENTRY    SESSION
CA SUBSCRIBER PRICE                                       0.00      -5.26

FILE 'CASREACT' ENTERED AT 08:08:40 ON 21 MAY 2007
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FILE CONTENT:1840 - 19 May 2007 VOL 146 ISS 22

New CAS Information Use Policies, enter HELP USAGETERMS for details.

*************************************************************
*                                                           *
*     CASREACT now has more than 12 million reactions       *
*                                                           *
*************************************************************

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provided by InfoChem, INPI data prior to 1986, and Biotransformations
database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance
identification.

=>
Uploading C:\Program Files\Stnexp\Queries\10553394-imideMg.str

L20     STRUCTURE UPLOADED

=>
Uploading C:\Program Files\Stnexp\Queries\10553394-imideNa.str

L21     STRUCTURE UPLOADED

=> d his

     (FILE 'HOME' ENTERED AT 06:49:26 ON 21 MAY 2007)

     FILE 'REGISTRY' ENTERED AT 06:49:47 ON 21 MAY 2007
                ACT INC553394/A
               ---------
L1              STR
L2           804 SEA FILE=REGISTRY SSS FUL L1
               ---------
L3              STRUCTURE UPLOADED
```

```
L4              STRUCTURE UPLOADED
L5          727 S L4 SSS FULL SUB=L2
                SAV TEM IN6553394/A L5
L6            7 S L3 SSS FULL SUB=L2

     FILE 'CAPLUS' ENTERED AT 06:51:56 ON 21 MAY 2007
L7          236 S L5
L8            3 S L6

     FILE 'STNGUIDE' ENTERED AT 06:52:38 ON 21 MAY 2007

     FILE 'CASREACT' ENTERED AT 07:17:13 ON 21 MAY 2007
L9              STRUCTURE UPLOADED
L10           0 S L9
L11           4 S L9 SSS FULL

     FILE 'CASREACT' ENTERED AT 07:59:56 ON 21 MAY 2007
L12             STRUCTURE UPLOADED
L13           3 S L12

     FILE 'STNGUIDE' ENTERED AT 08:00:29 ON 21 MAY 2007

     FILE 'CASREACT' ENTERED AT 08:03:10 ON 21 MAY 2007
L14             STRUCTURE UPLOADED
L15           1 S L14
L16         106 S L12 SSS FULL
                SAV TEM 3PR553394/A L16 IMI553394/A
                ACT IMI553394/A
               ---------
L17             STR
L18         106 SEA FILE=CASREACT SSS FUL L17 (   799 REACTIONS)
               ---------
L19          37 S L14 SSS FULL SUB=L18

     FILE 'STNGUIDE' ENTERED AT 08:06:08 ON 21 MAY 2007

     FILE 'CASREACT' ENTERED AT 08:08:40 ON 21 MAY 2007
L20             STRUCTURE UPLOADED
L21             STRUCTURE UPLOADED

=> s (l20 or l21) sub=l19 sss full
FULL SUBSET SEARCH INITIATED 08:09:54 FILE 'CASREACT'
SCREENING COMPLETE -       91 REACTIONS TO VERIFY FROM       19 DOCUMENTS

100.0% DONE      91 VERIFIED      91 HIT RXNS                      19 DOCS
SEARCH TIME: 00.00.01

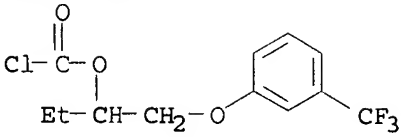
L22          19 SEA SUB=L19 SSS FUL (L20 OR L21) (    91 REACTIONS)

=> d scan

L22  19 ANSWERS   CASREACT  COPYRIGHT 2007 ACS on STN

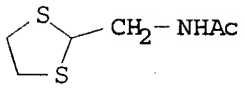
TI   Preparation of sulfur-containing heterocycle carbamate derivatives as
     herbicides
```

RX(7) OF 9



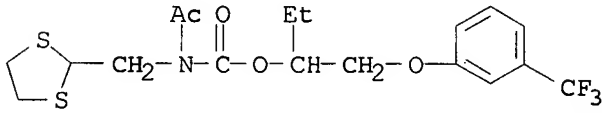
(step 2)

+



(step 1)

1. NaH, DMF
2. NaI



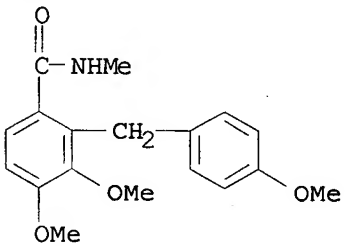
NOTE: ice-temp. for 1 h; ice-temp. for 10 min and room temp. for 1 h

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):18

L22 19 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

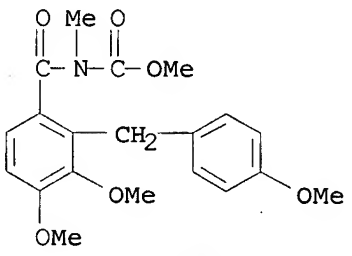
TI Niobium pentachloride promoted conversion of carboxylic acids to carboxamides: Synthesis of the 4-aryl-1,2,3,4-tetrahydroisoquinoline alkaloid structures

RX(39) OF 44



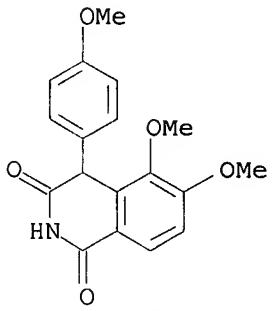
(step 1)

1. THF
2. BuLi, Hexane
3. ClCO2Me, THF
4. NaHCO3



31%

+

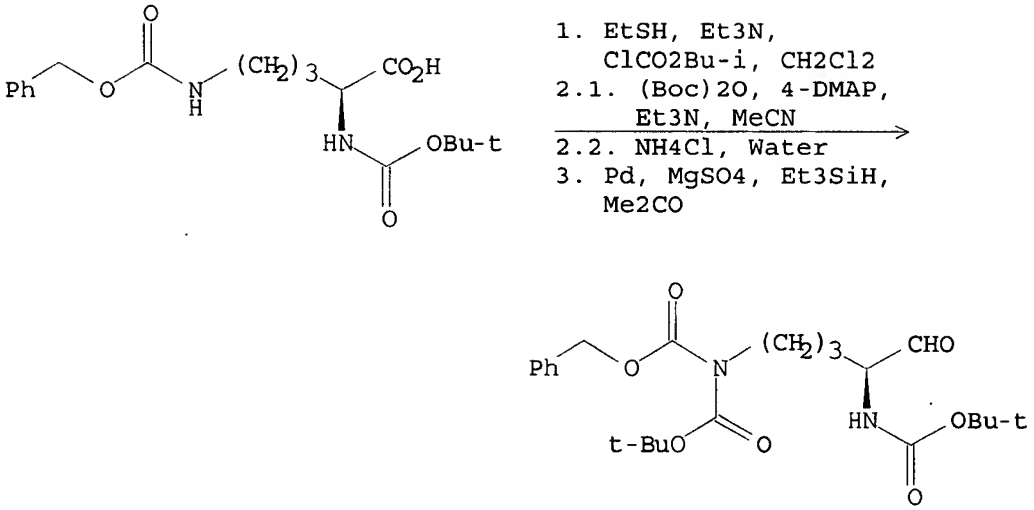


30%

L22 19 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Stereoselective Synthesis of Protected (2R,3R,4S)-4,7-Diamino-2,3-dihydroxyheptanoic Acid: A Novel Amino Acid of Callipeltins A and D

RX(26) OF 45 - 3 STEPS

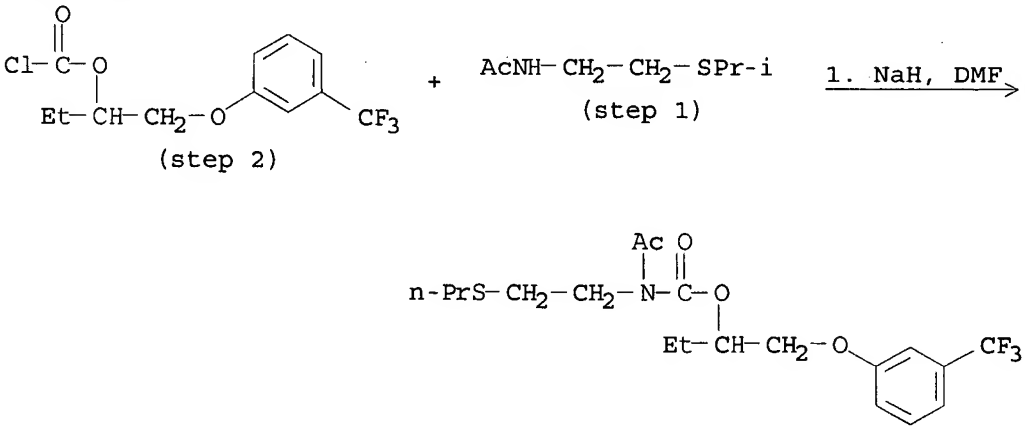


NOTE: 3) solid-supported catalyst

L22 19 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Preparation of acyl-substituted carbamates and herbicides comprising them

RX(3) OF 4

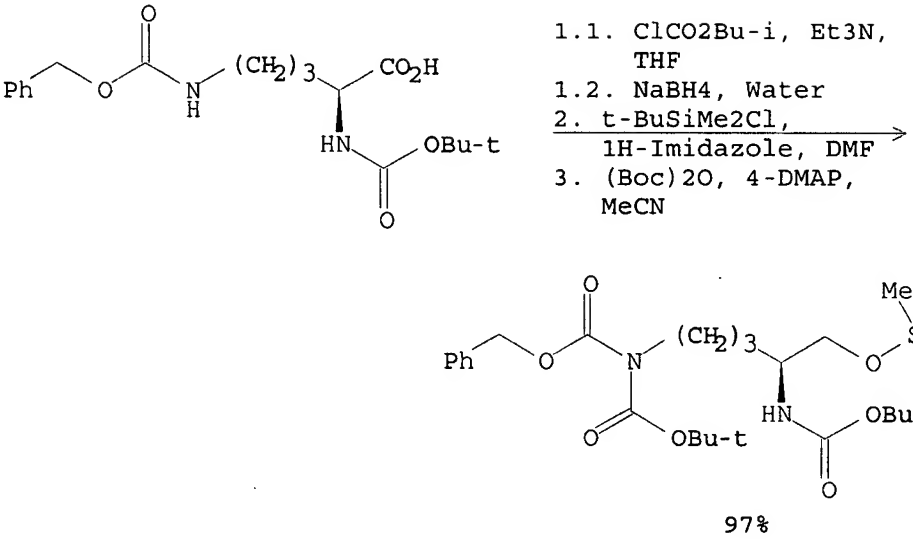


NOTE: ice-cooling for 1 h; ice-cooling for 10 min and room temp. for 2 h

L22 19 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Synthesis of the Unnatural Amino Acid AGDHE, a Constituent of the Cyclic Depsipeptides Callipeltins A and D

RX(42) OF 133 - 3 STEPS



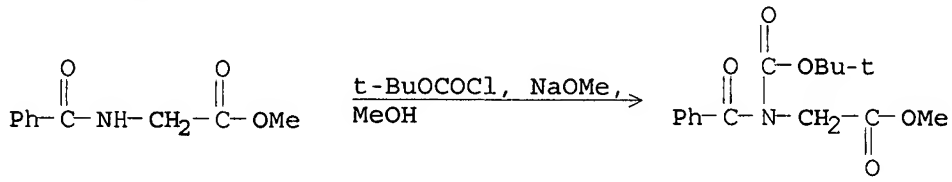
97%

NOTE: 3) regioselective

L22 19 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Observations on the reactivity of thiyl radicals derived from 3,6-epidithiodiketopiperazine-2,5-diones and related congeners

RX(10) OF 20

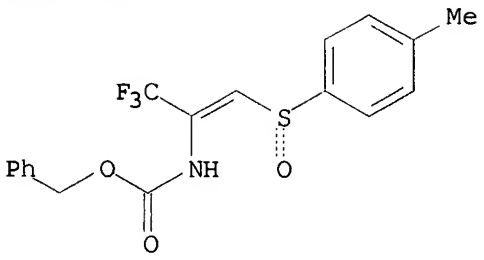


64%

L22 19 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

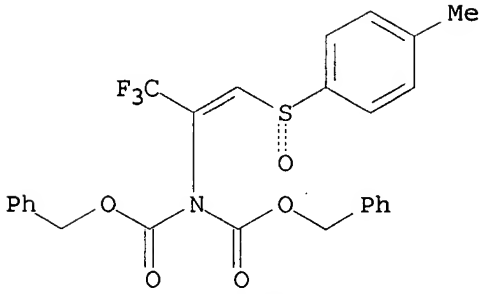
TI New Versatile Fluorinated Chiral Building Blocks: Synthesis and Reactivity of Optically Pure α-(Fluoroalkyl)-β-sulfinylenamines

RX(3) OF 53



1. NaH, DMF
2. ClCO2CH2Ph, DMF

(step 1)



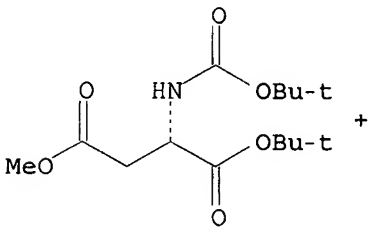
54%

NOTE: regioselective

L22 19 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Aspartyl phosphonates and phosphoramidates: the first synthetic inhibitors of bacterial aspartate-semialdehyde dehydrogenase

RX(60) OF 420 - 3 STEPS



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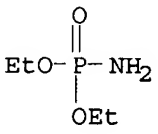
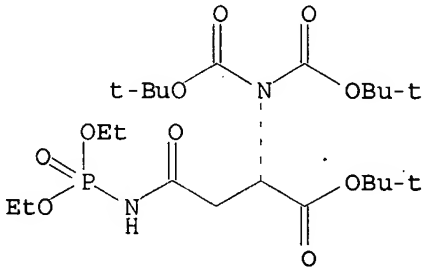


Li

(step 3.2)

1. (Boc)2O, NaH, THF
2. KOH, Water, MeCN
3.1. ClCO2Et, CH2Cl2
3.2. BuLi, CH2Cl2
3.3. HCl, Water



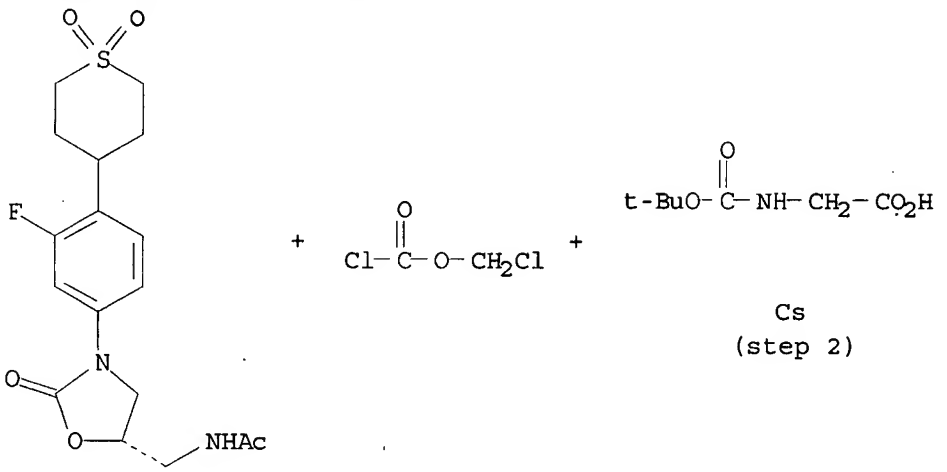
49%

L22 19 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

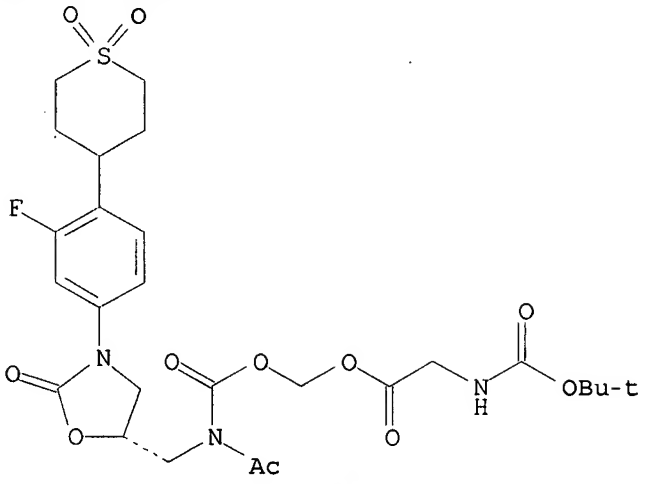
TI Preparation of acyloxymethyl carbamate prodrugs of oxazolidinone

bactericides with excellent oral bioavailability

RX(145) OF 413 - 2 STEPS



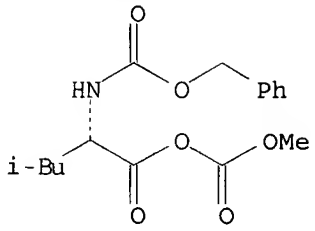
RX(145) OF 413 - 2 STEPS



L22 19 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

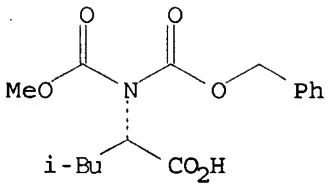
TI N,N-dialkoxycarbonylamino acids from the sodium hydride-mediated reaction of alkyl chloroformates with mixed anhydrides of N-alkoxycarbonylamino acids

RX(1) OF 2



1. ClCO2Me, NaH, MeCN
2. HCl, Water, MeOH

(step 1)

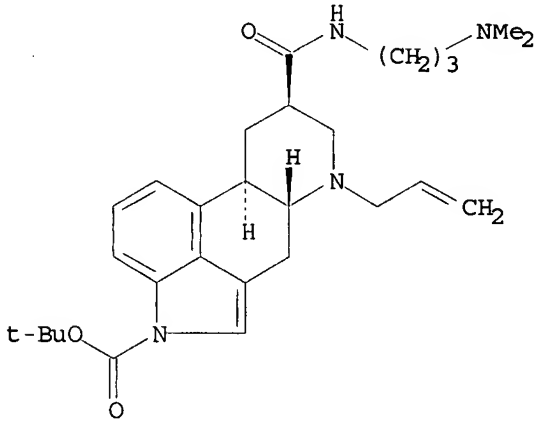


40%

L22 19 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI A Practical Synthesis of Cabergoline

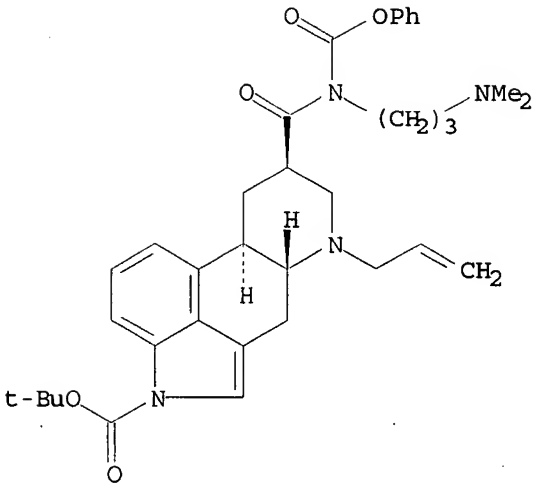
RX(4) OF 15



1. (Me3Si)2N.Na, THF
2. PhOCOCl

(step 1)

RX(4) OF 15

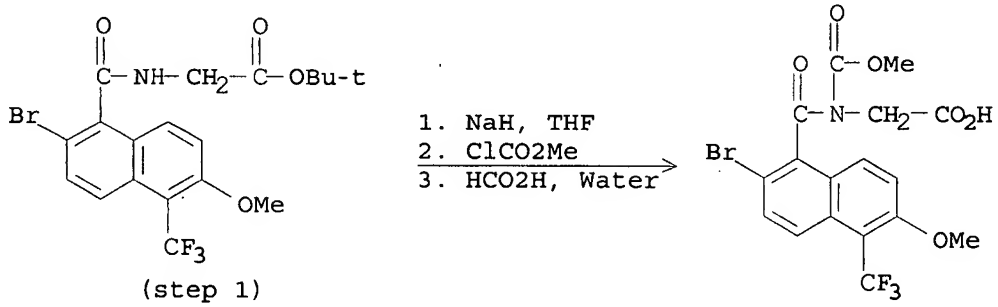


95%

L22 19 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Identification of [(naphthalene-1-carbonyl)-amino]-acetic acid derivatives as nonnucleoside inhibitors of HCV NS5B RNA dependent RNA polymerase

RX(8) OF 141

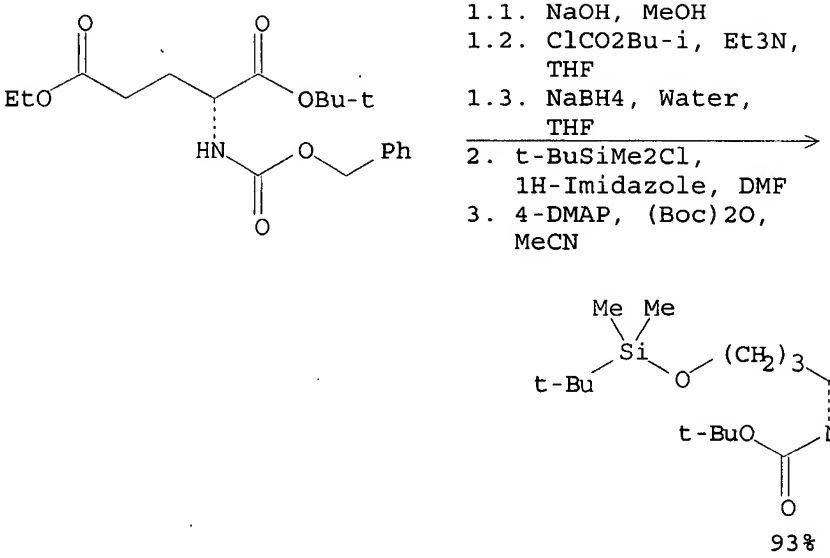


(step 1)

L22 19 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI 1-Hydroxy-3-amino-2-piperidone (δ-N-hydroxycycloornithine) derivatives: key intermediates for the synthesis of hydroxamate-based siderophores

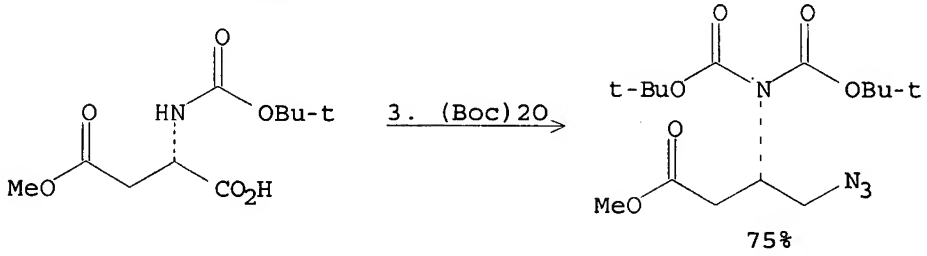
RX(146) OF 359 - 3 STEPS



L22 19 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI A novel approach to the synthesis of chiral terminal 1,2-diamines

RX(36) OF 72 - 3 STEPS

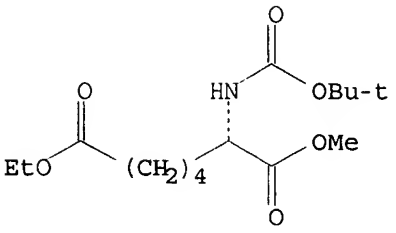


NOTE: 1) stereoselective, 2) stereoselective, 3) stereoselective

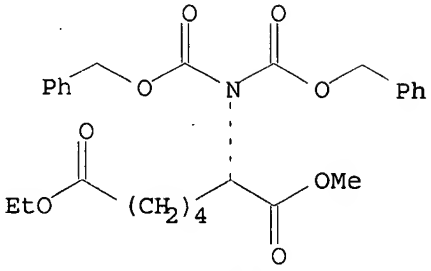
L22 19 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI First Practical Protection of α-Amino Acids as N,N-Benzyloxycarbamoyl Derivatives

RX(25) OF 28 - 2 STEPS



1.1. HCl, Water, THF, CH2Cl2
1.2. ClCO2CH2Ph, NaHCO3, Water
2.1. (Me3Si)2N.Li, HMPT, THF
2.2. ClCO2CH2Ph
2.3. NH4Cl, Water



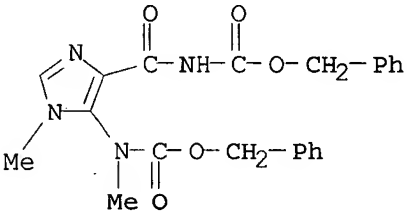
81%

NOTE: 2) alternative prepn. shown

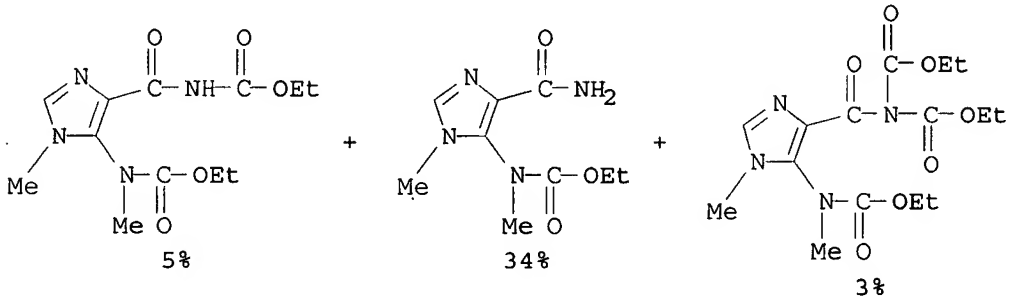
L22 19 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI 3-Methylxanthosine: synthesis and acidic hydrolysis of the glycosyl bond

RX(14) OF 25 - 2 STEPS



1. Pd, H2, EtOH
2. ClCO2Et, NaHCO3, Water

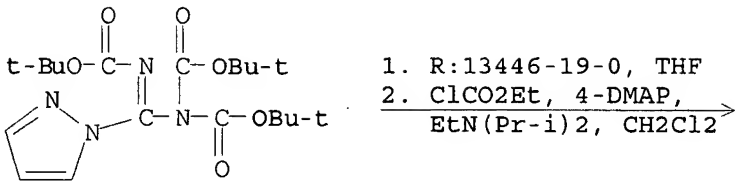


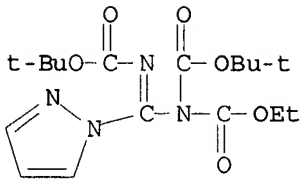
5% + 34% + 3%

L22 19 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Process for the preparation of butoxycarbonylimino compounds and intermediates therefor

RX(15) OF 28 - 2 STEPS



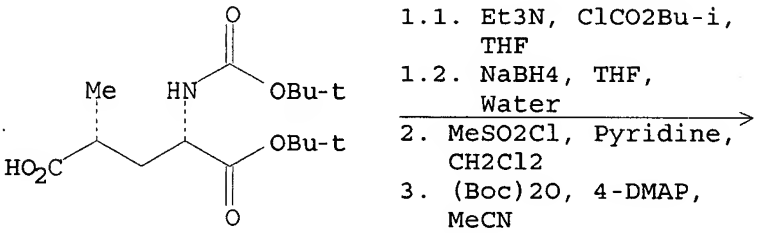


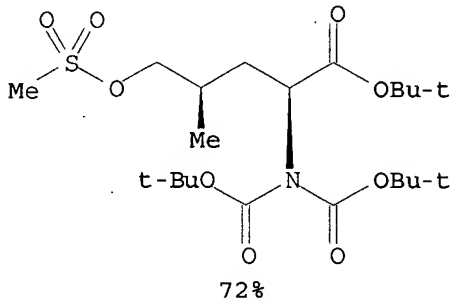
NOTE: 1) alternative prepn. shown, 2) other analogs similarly prepd.

L22 19 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Synthesis of (2S,4S)- and (2S,4R)-5-fluoroleucine and (2S,4S)-[5,5-2H2]-5-fluoroleucine

RX(59) OF 69 - 3 STEPS



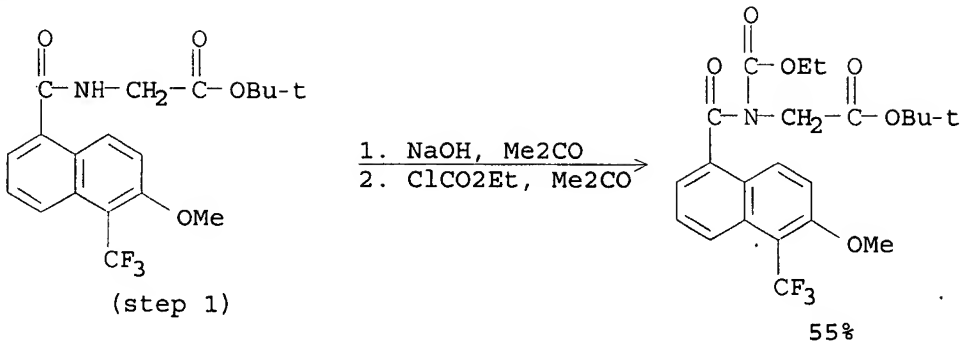


72%

L22 19 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Orally active aldose reductase inhibitors derived from bioisosteric substitutions on tolrestat

RX(36) OF 156



(step 1)

55%

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FULL ESTIMATED COST	16.05	394.48

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-5.26

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LAST RELOADED: May 18, 2007 (20070518/UP).

=> fil casreact

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.36	394.84

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CA SUBSCRIBER PRICE	0.00	-5.26

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FILE CONTENT:1840 - 19 May 2007 VOL 146 ISS 22

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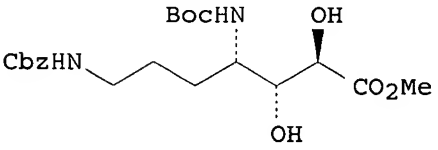
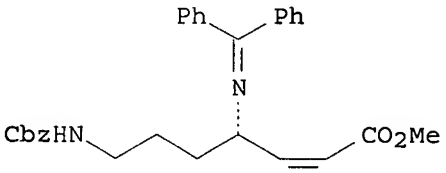
This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d cbib tot abs

L22 ANSWER 1 OF 19 CASREACT COPYRIGHT 2007 ACS on STN
144:468406 Stereoselective Synthesis of Protected (2R,3R,4S)-4,7-Diamino-2,3-dihydroxyheptanoic Acid: A Novel Amino Acid of Callipeltins A and D. Jeon, Jongho; Hong, Suk-Koo; Oh, Joon Seok; Kim, Young Gyu (School of Chemical and Biological Engineering, Seoul National University, Seoul, 151-744, S. Korea). Journal of Organic Chemistry, 71(8), 3310-3313 (English) 2006. CODEN: JOCEAH. ISSN: 0022-3263. Publisher: American Chemical Society.
GI



I



II

AB An orthogonally protected derivative I of (2R,3R,4S)-4,7-diamino-2,3-dihydroxyheptanoic acid, the unusual amino acid residue of the biol. active marine peptides such as callipeltins A and D and neamphamide A, was efficiently prepared in 10 steps and 30% overall yield from com. available Boc-Orn(Cbz)-OH. The key step includes the N-diphenylmethylene-controlled diastereoselective dihydroxylation of Cbz-ester II with >13:1 selectivity for the desired isomer.

L22 ANSWER 2 OF 19 CASREACT COPYRIGHT 2007 ACS on STN
143:43858 Observations on the reactivity of thiyl radicals derived from 3,6-epidithiodiketopiperazine-2,5-diones and related congeners. Hilton, S. T.; Motherwell, W. B.; Potier, P.; Pradet, C.; Selwood, D. L. (Chemistry Department, Christopher Ingold Laboratories, University College London, London, WC1H OAJ, UK). Bioorganic & Medicinal Chemistry Letters, 15(9), 2239-2242 (English) 2005. CODEN: BMCLE8. ISSN: 0960-894X. Publisher: Elsevier B.V..
AB A range of thiyl radicals derived from the reduced form of epidithiodiketopiperazines (ETPs) act as polarity reversal catalysts for the hydrosilylation of an enol lactone but not for H-atom abstraction from a model ribose ester.

L22 ANSWER 3 OF 19 CASREACT COPYRIGHT 2007 ACS on STN
142:355257 Preparation of acyloxymethyl carbamate prodrugs of oxazolidinone bactericides with excellent oral bioavailability. Josyula, Vara Prasad Venkata Nagendra; Gadwood, Robert C.; Thomasco, Lisa Marie; Kim, Ji-Young; Choy, Allison Laura; Boyer, Frederick Earl, Jr. (Pharmacia & Upjohn Company, USA). PCT Int. Appl. WO 2005028473 A1 20050331, 85 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB,

GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2004-IB2983 20040913. PRIORITY: US 2003-505329P 20030923.

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The present invention relates to acyloxymethyl carbamate oxazolidinones (shown as I; variables defined below; e.g. [[[N-acetyl[[(5R)-3-[4-(1,1-dioxidotetrahydro-2H-thiopyran-4-yl)-3-fluorophenyl]-2-oxo-1,3-oxazolidin-5-yl]methyl]amino]carbonyl]oxy]methyl acetate (shown as II)). These compds. have potent activity with excellent oral bioavailability against Gram-pos. and Gram-neg. bacteria. The single-dose pharmacokinetics of II and its parent compound are tabulated. For I: X is -SO-, -SO2-, or -SONR6-; Z is -C-, -CH-, or -N-; each dotted line = nothing or a bond; each W = -CHR6-, -CHR6CH2-, or nothing; R1 is -NH2, -NHC1-4alkyl, -C1-6alkyl, (un)substituted with 1-3 halo, -C2-6alkenyl, -(CH2)nC(O)C1-4alkyl, -OC1-4-alkyl, -SC1-4alkyl, or -(CH2)nC3-7cycloalkyl; R2 and R3 = -H, or -F; R4 is -H, -C1-4alkyl, or -CO2R6; R5 is -C1-10alkyl, -C3-7cycloalkyl, -aryl, -het, 1-OC1-10alkyl, -OC3-7cycloalkyl, -O-aryl, -O-het, -C(R6)(R7)NH2, -C(R6)(R7)NHCO2C1-4alkyl, -C(R6)(R7)NHCOC(R6)(R7)NH2, or -C(R6)(R7)NHCOC(R6)(R7)NHCO2C1-4alkyl; each R6 = -H, or -C1-4alkyl; each R7 = -H, -C1-4alkyl (C1-4alkyl = (un)substituted with OR6, SR6, CO2R6, CONH2, NH2, NHC(:NH)NH2, Ph, het, or R6 and R7 taken together form heterocycle); addnl. details are given in the claims. Although the methods of preparation are not claimed, .apprx.40 example prepns. are included. For example, II was prepared in 6 steps (72, 93, 55, , 85, and 78 % yields) starting from chloromethyl chloroformate and ethanethiol and involving intermediates carbonothioic acid O-(chloromethyl) S-Et ester, carbonothioic acid S-Et O-(iodomethyl) ester, carbonothioic acid O-[(acetyloxy)methyl] S-Et ester, carbonochloridic acid (acetyloxy)methyl ester, and [[[[[(5S)-3-[4-(1,1-dioxidotetrahydro-2H-thiopyran-4-yl)-3-fluorophenyl]-2-oxo-1,3-oxazolidin-5-yl]methyl]amino]carbonyl]oxy]methyl acetate.

L22 ANSWER 4 OF 19 CASREACT COPYRIGHT 2007 ACS on STN
141:253652 Identification of [(naphthalene-1-carbonyl)-amino]-acetic acid derivatives as nonnucleoside inhibitors of HCV NS5B RNA dependent RNA polymerase. Gopalsamy, Ariamala; Lim, Kitae; Ellingboe, John W.; Krishnamurthy, Girija; Orlowski, Mark; Feld, Boris; van Zeijl, Marja; Howe, Anita Y. M. (Chemical and Screening Sciences, Wyeth Research, Pearl River, NY, 10965, USA). Bioorganic & Medicinal Chemistry Letters, 14(16), 4221-4224 (English) 2004. CODEN: BMCLE8. ISSN: 0960-894X. Publisher: Elsevier Science B.V..

AB A novel series of HCV NS5B RNA dependent RNA polymerase inhibitors containing a naphthalene carboxamide scaffold were identified by high throughput screening. Optimization of substituents by parallel synthesis and the iterative design towards understanding structure-activity relationship to improve potency are described. Tetra substituted naphthalene 31 displayed potent activity with IC50 of 120 nM against HCV NS5B enzyme and was selective over a panel of polymerases.

L22 ANSWER 5 OF 19 CASREACT COPYRIGHT 2007 ACS on STN
141:23872 First Practical Protection of α-Amino Acids as N,N-Benzyloxycarbamoyl Derivatives. Hernandez, J. Nicolas; Martin, Victor

S. (Instituto Universitario de Bio-Organica "Antonio Gonzalez", Universidad de La Laguna, La Laguna, 38206, Spain). Journal of Organic Chemistry, 69(10), 3590-3592 (English) 2004. CODEN: JOCEAH. ISSN: 0022-3263. Publisher: American Chemical Society.

AB The consecutive treatment of N-Cbz amino protected compds. with LiHMDS and CbzCl provides a practical method for the preparation of N,N-di-Cbz derivs. in good yields. When α-amino acids are used the protection occurs without racemization. The method is compatible with a wide range of other functional and protecting groups. The procedure is also valid for the synthesis of mixed N,N-carbamoyl derivs.

L22 ANSWER 6 OF 19 CASREACT COPYRIGHT 2007 ACS on STN

140:391462 Synthesis of (2S,4S)- and (2S,4R)-5-fluoroleucine and (2S,4S)-[5,5-2H2]-5-fluoroleucine. Charrier, Jean-Damien; Hadfield, David S.; Hitchcock, Peter B.; Young, Douglas W. (Sussex Centre for Biomolecular Design and Drug Discovery, Department of Chemistry, University of Sussex, Brighton, BN1 9QJ, UK). Organic & Biomolecular Chemistry, 2(4), 474-482 (English) 2004. CODEN: OBCRAK. ISSN: 1477-0520. Publisher: Royal Society of Chemistry.

AB Syntheses of (2S,4S)- and (2S,4R)-5-fluoroleucine (1a and 2) and of (2S,4S)-[5,5-2H2]-5-fluoroleucine have been completed. The methodol. allows these compds. to be prepared in sufficient quantities for incorporation by solid-state protein synthesis into strategic sites in proteins for folding studies. X-ray structures of the epimers 1a and 2 have been obtained and show the presence of conformational isomerism. The torsion angles between the F-C bond and the main chain are compared with values found in a mutant of the protein ubiquitin in which (2S,4S)-5-fluoroleucine replaces leucine residues 50 and 67 in the native protein.

L22 ANSWER 7 OF 19 CASREACT COPYRIGHT 2007 ACS on STN

138:385601 Niobium pentachloride promoted conversion of carboxylic acids to carboxamides: Synthesis of the 4-aryl-1,2,3,4-tetrahydroisoquinoline alkaloid structures. Nery, Marcelo S.; Ribeiro, Renata P.; Lopes, Claudio C.; Lopes, Rosangela S. C. (Instituto de Quimica, Departamento de Quimica Analitica, Universidade Federal do Rio de Janeiro, Instituto de Quimica, Departamento de Quimica Analitica, CT,, Bl. A, 5° andar, s-508, Rio de Janeiro, CEP-21949 900, Brazil). Synthesis (2), 272-276 (English) 2003. CODEN: SYNTBF. ISSN: 0039-7881. Publisher: Georg Thieme Verlag.

AB A practical method for the conversion of carboxylic acids to the corresponding carboxamides mediated by niobium pentachloride under mild conditions is described. The synthesis of the 4-aryl-1,2,3,4-tetrahydroisoquinoline alkaloid structures was accomplished via benzylic lithiation of N-methyl-3,4-dimethoxy-2-(4'-methoxybenzyl)benzamide.

L22 ANSWER 8 OF 19 CASREACT COPYRIGHT 2007 ACS on STN

138:106962 Synthesis of the Unnatural Amino Acid AGDHE, a Constituent of the Cyclic Depsipeptides Callipeltins A and D. Thoen, Jason C.; Morales-Ramos, Angel I.; Lipton, Mark A. (Department of Chemistry, Purdue University, West Lafayette, IN, 47907-1393, USA). Organic Letters, 4(25), 4455-4458 (English) 2002. CODEN: ORLEF7. ISSN: 1523-7060. Publisher: American Chemical Society.

AB The novel amino acid residue (2R,3R,4S)-4-amino-7-guanidino-2,3-dihydroxyheptanoic acid (AGDHE; an amino acid of the cyclic depsipeptides callipeltins A and D), and its (2S,3S,4S) diastereomer were synthesized from a protected L-ornithine derivative, Boc-Orn(Cbz)-OH, in 13 steps (15% overall yield). Configurational assignment of AGDHE was reexamd. by 1H NMR.

L22 ANSWER 9 OF 19 CASREACT COPYRIGHT 2007 ACS on STN

138:68805 Aspartyl phosphonates and phosphoramidates: the first synthetic inhibitors of bacterial aspartate-semialdehyde dehydrogenase. Cox, Russell J.; Gibson, Jennifer S.; Martin, Maria Belen Mayo (School of Chemistry, University of Bristol, Bristol, BS8 1AS, UK). ChemBioChem, 3(9), 874-886 (English) 2002. CODEN: CBCHFX. ISSN: 1439-4227. Publisher: Wiley-VCH Verlag GmbH.

AB The synthesis of methylene phosphonate, difluoromethylene phosphonate and phosphoramidate analogs of aspartyl phosphate, together with reduced analogs, is described. These compds. were shown to be effective inhibitors of aspartate-semialdehyde dehydrogenase (ASA-DH) from Escherichia coli. However, despite the structural similarity of the compds., different patterns of inhibition were observed, indicative of two phases of recognition and binding. Correlation between measured inhibition consts. with pKa values supports the theory that binding at the phosphate binding site is optimized for singly ionized phosphate analogs.

L22 ANSWER 10 OF 19 CASREACT COPYRIGHT 2007 ACS on STN

137:353201 A Practical Synthesis of Cabergoline. Ashford, Scott W.; Henegar, Kevin E.; Anderson, Andrew M.; Wuts, Peter G. M. (Chemical Process Research and Development, Pharmacia Corporation, Kalamazoo, MI, 49001, USA). Journal of Organic Chemistry, 67(20), 7147-7150 (English) 2002. CODEN: JOCEAH. ISSN: 0022-3263. Publisher: American Chemical Society.

AB Cabergoline is an N-acylurea derived from 9,10-dihydrolyzergic acid, which is a potent prolactin inhibitor. It is marketed by Pharmacia as Dostinex for the treatment of hyperprolactinemia and is currently under active development for the treatment of a variety of CNS disorders. In the existing process, the N-acylurea is formed by the reaction of an amide with a large excess of Et isocyanate at elevated temps. An improved process was developed that eliminates this hazardous reaction. The amide is reacted with Ph chloroformate and then with ethylamine, which provides a mild and efficient means of forming the unsym. N-acylurea.

L22 ANSWER 11 OF 19 CASREACT COPYRIGHT 2007 ACS on STN

134:237196 A novel approach to the synthesis of chiral terminal 1,2-diamines. Markidis, Theodoros; Kokotos, George (Laboratory of Organic Chemistry Department of Chemistry, University of Athens, Panepistimiopolis Athens, 15771, Greece). Journal of Organic Chemistry, 66(5), 1919-1923 (English) 2001. CODEN: JOCEAH. ISSN: 0022-3263. Publisher: American Chemical Society.

AB The authors have developed a novel general method for the synthesis of enantiomerically pure 1,2-diamines, e.g., (2S,5Z)-RCH:CH(CH2)2CH(NH2)CH2NH2·(HCl)2, using the aldehydes (2S)-OHC(CH2)nCH(NBoc2)CH2N3 (I, n = 1, 2), as key intermediates. I were coupled with phosphorus ylides to give unsatd. azides, which were reduced to amines. The strengths of the method are in its (1) simplicity and efficiency; (2) flexibility with respect to the substituent groups that can be introduced through the olefination reaction and the chirality of the product, which depends on the chirality of Glu or Asp; and (3) applicability to the development of new 1,2-diamines with desired target structures for biol. studies.

L22 ANSWER 12 OF 19 CASREACT COPYRIGHT 2007 ACS on STN

134:56663 Process for the preparation of butoxycarbonylimino compounds and intermediates therefor. Dowle, Michael Dennis; Howes, Peter David; Robinson, John Edward; Trivedi, Naimish (Glaxo Group Limited, UK). PCT Int. Appl. WO 2000078723 A1 20001228, 27 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM;

RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 2000-GB2355 20000616. PRIORITY: GB 1999-14306 19990619.

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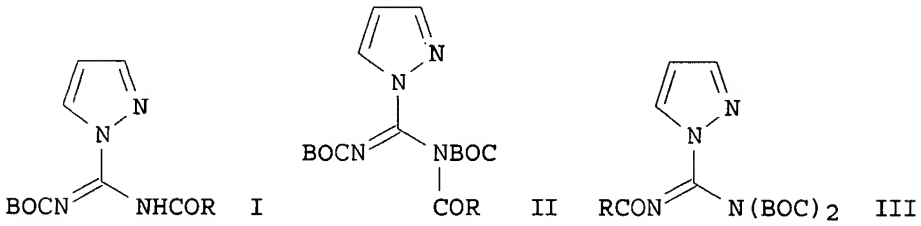

AB Pyrazole derivs. I (R = alkyl, aryl, alkoxy, aryloxy, amino acid residue, etc.) were prepared by treatment of intermediates II or III (same R) with a metal salt such as Mg(ClO4)·6H2O (IV). Thus, 11 g of IV was added to a stirred suspension of 195 g of III (R = Me3CO), and the mixture was stirred and warmed to 45°, then maintained at 50° for 2 h to give 118 g of I (same R).

L22 ANSWER 13 OF 19 CASREACT COPYRIGHT 2007 ACS on STN
132:279222 Preparation of sulfur-containing heterocycle carbamate derivatives as herbicides. Chiba, Yutaka; Matsuno, Hiromi; Ozawa, Shuji; Eda, Sadafumi; Hirase, Kangetsu (Mitsui Chemicals Inc., Japan). Jpn. Kokai Tokkyo Koho JP 2000109477 A 20000418, 42 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1998-283067 19981005.

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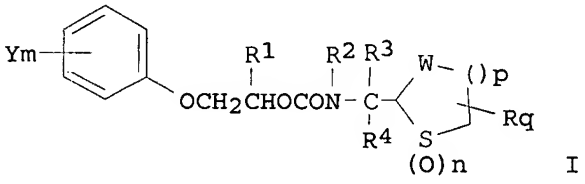

AB The title compds. (I; R-R4 = H, C1-4 alkyl, cycloalkyl; W = NH, O, S, SO, SO2; Y = C1-4 alkyl, cycloalkyl, haloalkyl, alkoxy, haloalkoxy, alkylthio, haloalkylthio, alkylsulfinyl, haloalkylsulfinyl, alkylsulfonyl, haloalkylsulfonyl, alkylsulfonamido, haloalkylsulfonamido, halo, acyl, cyano, NO2; m = 1,2; n = 0-2; q = 1-3) are prepared via several synthetic routes. These compds. are quite safe and exhibit excellent herbicidal activity against weeds of rice paddy and upland. Thus, (1,3-oxathian-2-yl)methylamine was added to a solution of 2-[(imidazol-1-ylcarbonyl)oxy]-1-[3-(trifluoromethyl)phenoxy]butane in THF and stirred at 60° for 12 h to give 2-[N-[(1,3-oxathian-2-yl)methyl]carbamoyloxy]-1-[3-(trifluoromethyl)phenoxy]butane (II). II at 0.3 kg/ha preemergence completely controlled Echinochloa crus-galli, Monochoria vaginalis, Scirpus juncoides, and Sagittaria pygmaean and did not damage rice seedlings.

L22 ANSWER 14 OF 19 CASREACT COPYRIGHT 2007 ACS on STN
132:137179 Preparation of acyl-substituted carbamates and herbicides comprising them. Matsuno, Hiromi; Chiba, Yutaka; Ozawa, Shuji; Eta, Sadafumi; Hirase, Kangetsu (Mitsui Chemicals Inc., Japan). Jpn. Kokai

Tokkyo Koho JP 2000038373 A 20000208, 85 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1998-205463 19980721.

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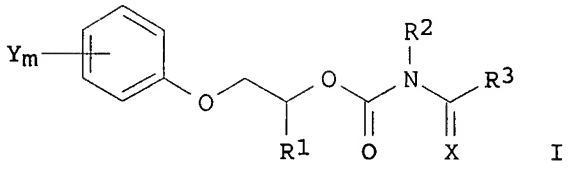

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AB Title compds. I (R1 = H, C1-4 alkyl, cycloalkyl; R2 = alkylthioalkyl, cycloalkylthioalkyl, alkenylthioalkyl, alkynylthioalkyl, etc.; X = O, S, NR6; R3, R6 = C1-4 alkyl, cycloalkyl, substituted Ph; Y = C1-4 alkyl, cycloalkyl, haloalkyl, alkoxy, etc.; m = 1-5) are prepared by, for instance, reaction of II (R1, R2, Y, m = same as I) with QC(X)R3 (R3, X = same as I; Q = leaving group). 2-[[N-[2-(methylthio)-1-ethyl]carbamoyl]oxy]-1-[3-(trifluoromethyl)phenoxy]butane (0.70 g) was reacted with 0.34 g benzoyl chloride in the presence of NaH in DMF at 4° to room temperature for 2.5 h to give 0.56 g 2-[[N-benzoyl-N-[2-(methylthio)-1-ethyl]carbamoyl]oxy]-1-[3-(trifluoromethyl)phenoxy]butane showing good herbicidal activity.

L22 ANSWER 15 OF 19 CASREACT COPYRIGHT 2007 ACS on STN

125:33255 New Versatile Fluorinated Chiral Building Blocks: Synthesis and Reactivity of Optically Pure α-(Fluoroalkyl)-β-sulfinylenamines. Arnone, Alberto; Bravo, Pierfrancesco; Capelli, Silvia; Fronza, Giovanni; Meille, Stefano V.; Zanda, Matteo; Cavicchio, Giancarlo; Crucianelli, Marcello (Dipartimento di Chimica, Politecnico Milano, Milan, I-20133, Italy). Journal of Organic Chemistry, 61(10), 3375-87 (English) 1996. CODEN: JOCEAH. ISSN: 0022-3263. Publisher: American Chemical Society.

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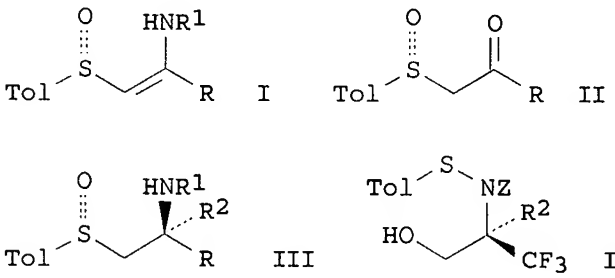

AB Efficient synthesis of optically pure α-(fluoroalkyl)-β-sulfinyl enamines I [Tol = 4-MeC6H4; R = CF3, CF2H, CF2Cl, CF2CF3, CFH2; R1 = H, CO2CH2Ph (Z)] has been achieved by aza-Wittig reaction of triphenyliminophosphoranes Ph2P:NR1 (R1 = Z, H, SiMe3) with the corresponding α-fluorinated-α'-sulfinyl ketones II. I showed an overwhelming preference for the Z stereochem. of the enamine form. Their general reactivity has been studied. The reaction with some electrophiles (i.e. benzyl chloroformate and benzyl and allyl bromide) occurs at the nitrogen atom providing the corresponding N,N-disubstituted enamines. Nucleophiles add smoothly to C-2: heteroatom-centered nucleophiles like methanol, ammonia, and thiophenol afford gem-disubstituted derivs. under thermodn. control, while a C-centered nucleophile like nitromethane adds in irreversible fashion. The hydride-

and deuteride-promoted reduction of I to α-fluorinated-α'-sulfinyl amines III (R2 = H, D) has been studied. Hydride addition was stereoselective, while low stereoselection was obtained with the other tested nucleophiles. Desulfurization of optically pure sulfinylamine III (R = CF3, R1 = R2 = H) afforded (R)-1-(trifluoromethyl)ethylamine. The Pummerer rearrangement of III (R = CF3, R1 = Z) occurs in an unusual nonoxidative way affording sulfenamides IV, that readily provided (R)-3,3,3-trifluoroalaninol and its 2-deutero analog, and (R)-3,3,3-trifluoroalanine.

L22 ANSWER 16 OF 19 CASREACT COPYRIGHT 2007 ACS on STN
123:170105 N,N-dialkoxycarbonylamino acids from the sodium hydride-mediated reaction of alkyl chloroformates with mixed anhydrides of N-alkoxycarbonylamino acids. Benoiton, N. Leo; Akyurekli, Deniz; Chen, Francis M. F. (Dep. Biochem., Univ. Ottawa, Ottawa, ON, Can.). International Journal of Peptide & Protein Research, 45(5), 466-70 (English) 1995. CODEN: IJPPC3. ISSN: 0367-8377. Publisher: Munksgaard.
AB Reaction of protected amino acid mixed anhydrides R1NHCHR2CO2CO2R3 (R1 = PhCH2O2C, Me3CO2C; R2 = Me, CHMe2, CH2CHMe2; R3 = Me, Et, CH2Ph, CH2CH:CH2) with NaH and chloroformates ClCO2R3 followed by acid hydrolysis gives modest yields of title compds. R3O2CNR1CHR2CO2H. The products are contaminated by parent acids R1NHCHR2CO2H that are not readily removed. Crossover expts. show that about 75% of the acylation originates from intramol. transfer of the alkyl carbonate moiety; the remainder comes from acylation by the alkyl chloroformate.

L22 ANSWER 17 OF 19 CASREACT COPYRIGHT 2007 ACS on STN
113:191866 1-Hydroxy-3-amino-2-piperidone (δ-N-hydroxycycloornithine) derivatives: key intermediates for the synthesis of hydroxamate-based siderophores. Kolasa, Teodozyj; Miller, Marvin J. (Dep. Chem., Univ. Notre Dame, Notre Dame, IN, 46556, USA). Journal of Organic Chemistry, 55(6), 1711-21 (English) 1990. CODEN: JOCEAH. ISSN: 0022-3263.
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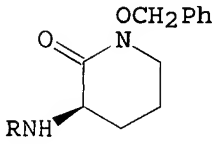

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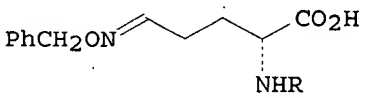

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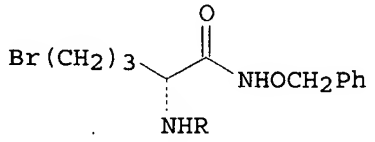

III

AB Several routes for the synthesis of δ-N-(benzyloxy)cycloornithine (I, R = CO2CH2Ph, CO2CH2CH:CH2, phthalimido) from glutamic acid-derived starting materials were developed. Efficient methods were developed for the synthesis of glutamic acid γ-semialdehyde and δ-hydroxynorvaline derivs. as key substrates for preparation of δ-N-hydroxyornithine analogs. Thus, the best approaches to the synthesis of I were reductive cyclization of an N-hydroxysuccinimide ester of the O-benzyloxime of α-amino-protected glutamic acid γ-semialdehyde (II) or cyclization of the N-(benzyloxy)amide of δ-bromonorvaline (III).

L22 ANSWER 18 OF 19 CASREACT COPYRIGHT 2007 ACS on STN
112:77811 3-Methylxanthosine: synthesis and acidic hydrolysis of the glycosyl bond. Itaya, Taisuke; Harada, Tsunehiro (Fac. Pharm. Sci., Kanazawa Univ., Takara, 920, Japan). Chemical & Pharmaceutical Bulletin, 37(5), 1235-8 (English) 1989. CODEN: CPBTAL. ISSN: 0009-2363.

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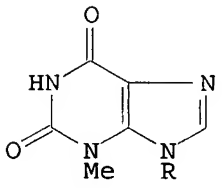

I

AB An improved synthesis of 3,9-dimethylxanthine (I; R = Me) was achieved via the reaction of 1-methyl-5-(methylamino)-imidazole-4-carboxamide with EtOCOCl in acetate buffer (pH 5) followed by treatment with aqueous NaOH. This method was successfully applied to the synthesis of 3-methylxanthosine (I; R = β-D-ribofuranosyl) (II), whose N-glycosidic bond proved to be remarkably sensitive to acidic hydrolysis: II underwent hydrolysis at a rate more than 1000 times faster than that of xanthosine in 1.0N aqueous HCl at 25°.

L22 ANSWER 19 OF 19 CASREACT COPYRIGHT 2007 ACS on STN
111:195363 Orally active aldose reductase inhibitors derived from bioisosteric substitutions on tolrestat. Wrobel, Jay; Millen, Jane; Sredy, Janet; Dietrich, Arlene; Kelly, Joseph M.; Gorham, Beverly J.; Sestanj, Kazimir (Wyeth-Ayerst Res. Inc., Princeton, NJ, 08543-8000, USA). Journal of Medicinal Chemistry, 32(11), 2493-500 (English) 1989. CODEN: JMCMAR. ISSN: 0022-2623.

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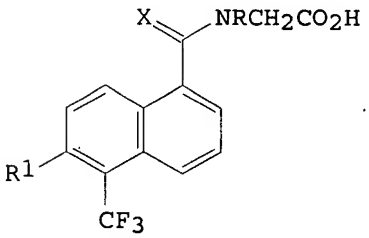

I

AB A series of aldose reductase inhibitors was prepared in which structural modifications were made to three positions of the potent, orally active inhibitor tolrestat (I, R = Me, R1 = OMe, X = S) (II), namely, the 6-methoxy substituent, thioamide S, and the N-Me moiety. These compds. were evaluated in two in vitro systems: an isolated enzyme preparation from bovine lens to assess their intrinsic inhibitory activity and an isolated rat sciatic nerve assay to determine their ability to penetrate membranes of nerve tissue. These compds. were also evaluated in vivo as inhibitors of galactitol accumulation in the lens, sciatic nerve, and diaphragm of galactose-fed rats. Bioisosteric replacement of the 6-methoxy group with a methylthio substituent gave I (R = Me, R1 = SMe, X = S) (III), and replacement of the thioamide substituent with a cyanoamidine gave I (R = Me, R1 = OMe, X = NCN) (IV). Both III and IV retained high in vitro potency but were less potent in vivo than II. Replacement of the N-Me

group by a carbomethoxy moiety gave I (R = CO2Me, R1 = OMe, X = S) and led to a substantial reduction in activity in each of the three assays employed. However, this same structural modification of oxotolrestat led to I (R = CO2Me, R1 = OMe, X = O) and resulted in an enhancement of the intrinsic activity and a comparable in vivo potency. The isolated nerve data suggest that some compds. in these series do not readily penetrate into peripheral nerves, and this presumably is a factor in their lack of oral activity.

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L2	84990	candida or humicola or mucor or pseudomonas or rhizopus or brevundimonas or cellulomonas or jensenia or rhodococcus or saccharamycopsis or trichosporon	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT; IBM_TDB	OR	ON	2007/05/21 13:38
L3	278	l1 and l2	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT; IBM_TDB	OR	ON	2007/05/21 13:38
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L7	22	l6 and l2 and l4	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT; IBM_TDB	OR	ON	2007/05/21 13:39

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 NEWS 20  MAR 20   MARPAT now updated daily
 NEWS 21  MAR 22   LWPI reloaded
 NEWS 22  MAR 30   RDISCLOSURE reloaded with enhancements
 NEWS 23  APR 02   JICST-EPLUS removed from database clusters and STN
 NEWS 24  APR 30   GENBANK reloaded and enhanced with Genome Project ID field
 NEWS 25  APR 30   CHEMCATS enhanced with 1.2 million new records
 NEWS 26  APR 30   CA/CAplus enhanced with 1870-1889 U.S. patent records
 NEWS 27  APR 30   INPADOC replaced by INPADOCDB on STN
 NEWS 28  MAY 01   New CAS web site launched
 NEWS 29  MAY 08   CA/CAplus Indian patent publication number format defined
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L1 STRUCTURE UPLOADED

=> s l1 sam
SAMPLE SEARCH INITIATED 14:43:03 FILE 'CASREACT'
SCREENING COMPLETE - 13140 REACTIONS TO VERIFY FROM 970 DOCUMENTS

38.1% DONE 5000 VERIFIED 95 HIT RXNS 2 DOCS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED VERIFICATIONS: 255992 TO 269608
PROJECTED ANSWERS: 2 TO 303

L2 2 SEA SSS SAM L1 (95 REACTIONS)

=> d scan

L2 2 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Synthesis of iso-epoxy-amphidinolide N and des-epoxy-caribenolide I structures. Revised strategy and final stages

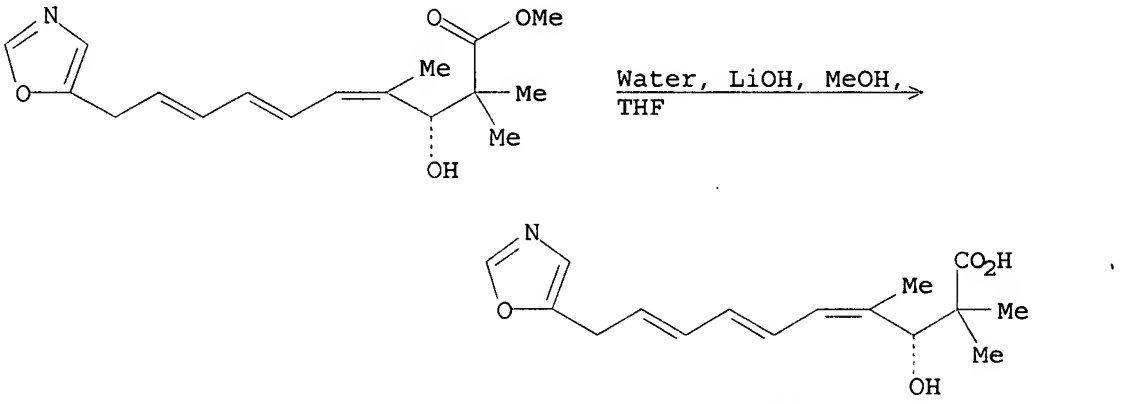
RX(38) OF 636 - REACTION DIAGRAM NOT AVAILABLE

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 2 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI A general route to the Streptomyces-derived inthomycin family: the first synthesis of (+)-inthomycin B

RX(12) OF 234



73%

ALL ANSWERS HAVE BEEN SCANNED

=> fil stng

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.90	1.11

FILE 'STNGUIDE' ENTERED AT 14:43:22 ON 21 MAY 2007
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FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: May 18, 2007 (20070518/UP).

=> fil casreact

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.12	1.23

FILE 'CASREACT' ENTERED AT 14:44:32 ON 21 MAY 2007
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FILE CONTENT:1840 - 19 May 2007 VOL 146 ISS 22

```
New CAS Information Use Policies, enter HELP USAGETERMS for details.

*************************************************************
*                                                           *
*     CASREACT now has more than 12 million reactions       *
*                                                           *
*************************************************************

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999)
provided by InfoChem, INPI data prior to 1986, and Biotransformations
database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance
identification.

=>
Uploading C:\Program Files\Stnexp\Queries\10553394-hydrolase2.str

L3      STRUCTURE UPLOADED

=> s l3 sam
SAMPLE SEARCH INITIATED 14:44:49 FILE 'CASREACT'
SCREENING COMPLETE -    13140 REACTIONS TO VERIFY FROM      970 DOCUMENTS

 38.1% DONE    5000 VERIFIED      40 HIT RXNS                        2 DOCS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS:    255992 TO   269608
PROJECTED ANSWERS:               2 TO      303

L4            2 SEA SSS SAM L3 (    40 REACTIONS)

=> d scan

L4   2 ANSWERS   CASREACT  COPYRIGHT 2007 ACS on STN

TI   Synthesis of iso-epoxy-amphidinolide N and des-epoxy-caribenolide I
     structures. Revised strategy and final stages

RX(38) OF 636 - REACTION DIAGRAM NOT AVAILABLE

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> fil stng
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                                 0.45       1.68

FILE 'STNGUIDE' ENTERED AT 14:45:01 ON 21 MAY 2007
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AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: May 18, 2007 (20070518/UP).

=> s l3 sss full
SUBSTANCE QUERIES NOT VALID IN THIS FILE
The logic expression entered contains L#s or saved query names which
correspond to structures built by the STRUCTURE command or to screen
```

sets. These must be searched in a substance file such as the REGISTRY file. In some files you may use a Registry Number answer set from a structure search as a search term or profile in some bibliographic file containing Registry Numbers, e.g. the CA file. For an explanation, enter "HELP CROSSOVER" at an arrow prompt (=>).

=> fil casreact
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 0.12 1.80

FILE 'CASREACT' ENTERED AT 14:46:27 ON 21 MAY 2007
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FILE CONTENT:1840 - 19 May 2007 VOL 146 ISS 22

New CAS Information Use Policies, enter HELP USAGETERMS for details.

****
* *
* CASREACT now has more than 12 million reactions *
* *
****

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3 sss full
FULL SEARCH INITIATED 14:46:30 FILE 'CASREACT'
SCREENING COMPLETE - 255666 REACTIONS TO VERIFY FROM 19193 DOCUMENTS

98.7% DONE 252245 VERIFIED 417 HIT RXNS (3 INCOMP) 146 DOCS

100.0% DONE 255666 VERIFIED 418 HIT RXNS (3 INCOMP) 147 DOCS
SEARCH TIME: 00.00.32

L5 147 SEA SSS FUL L3 (418 REACTIONS)

=> sav tem hyd553394/a
ENTER L#, L# RANGE, ALL, OR (END):l5

=> fil stng
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 114.00 115.80

FILE 'STNGUIDE' ENTERED AT 14:47:25 ON 21 MAY 2007
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FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: May 18, 2007 (20070518/UP).

```
=> fil casreact
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                         0.12     115.92

FILE 'CASREACT' ENTERED AT 14:48:54 ON 21 MAY 2007
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FILE CONTENT:1840 - 19 May 2007 VOL 146 ISS 22

New CAS Information Use Policies, enter HELP USAGETERMS for details.

************************************************************
*                                                          *
*     CASREACT now has more than 12 million reactions      *
*                                                          *
************************************************************

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999)
provided by InfoChem, INPI data prior to 1986, and Biotransformations
database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substancé
identification.

=>
Uploading C:\Program Files\Stnexp\Queries\10553394-hydrolase4.str

L6      STRUCTURE UPLOADED

=> s l6 sub=l5 sam
SAMPLE SUBSET SEARCH INITIATED 14:49:18 FILE 'CASREACT'
SCREENING COMPLETE -       50 REACTIONS TO VERIFY FROM        7 DOCUMENTS

100.0% DONE      50 VERIFIED       0 HIT RXNS                      0 DOCS
SEARCH TIME: 00.00.01

PROJECTIONS (WITHIN SPECIFIED SUBSET):          ONLINE  **COMPLETE**
PROJECTED VERIFICATIONS (WITHIN SPECIFIED SUBSET):     576 TO     1424
PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET):             0 TO        0

L7            0 SEA SUB=L5 SSS SAM L6 (     0 REACTIONS)

=> s l6 sub=l5 sss full
FULL SUBSET SEARCH INITIATED 14:49:27 FILE 'CASREACT'
SCREENING COMPLETE -      418 REACTIONS TO VERIFY FROM      147 DOCUMENTS

100.0% DONE     418 VERIFIED      61 HIT RXNS (     1 INCOMP)       27 DOCS
SEARCH TIME: 00.00.01

L8           27 SEA SUB=L5 SSS FUL L6 (    61 REACTIONS)

=> d his

     (FILE 'HOME' ENTERED AT 14:42:13 ON 21 MAY 2007)

     FILE 'CASREACT' ENTERED AT 14:42:21 ON 21 MAY 2007
L1              STRUCTURE UPLOADED
```

```
L2             2 S L1 SAM

     FILE 'STNGUIDE' ENTERED AT 14:43:22 ON 21 MAY 2007

     FILE 'CASREACT' ENTERED AT 14:44:32 ON 21 MAY 2007
L3               STRUCTURE UPLOADED
L4             2 S L3 SAM

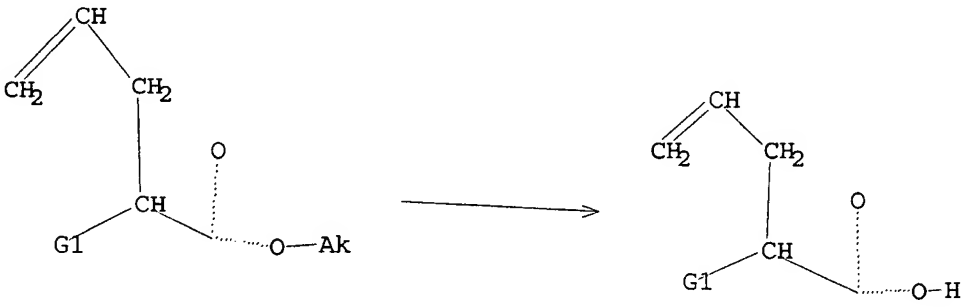
     FILE 'STNGUIDE' ENTERED AT 14:45:01 ON 21 MAY 2007

     FILE 'CASREACT' ENTERED AT 14:46:27 ON 21 MAY 2007
L5           147 S L3 SSS FULL
                 SAV TEM HYD553394/A L5

     FILE 'STNGUIDE' ENTERED AT 14:47:25 ON 21 MAY 2007

     FILE 'CASREACT' ENTERED AT 14:48:54 ON 21 MAY 2007
L6               STRUCTURE UPLOADED
L7             0 S L6 SAM SUB=L5
L8            27 S L6 SSS FULL SUB=L5

=> d l6
L6 HAS NO ANSWERS
L6               STR
```

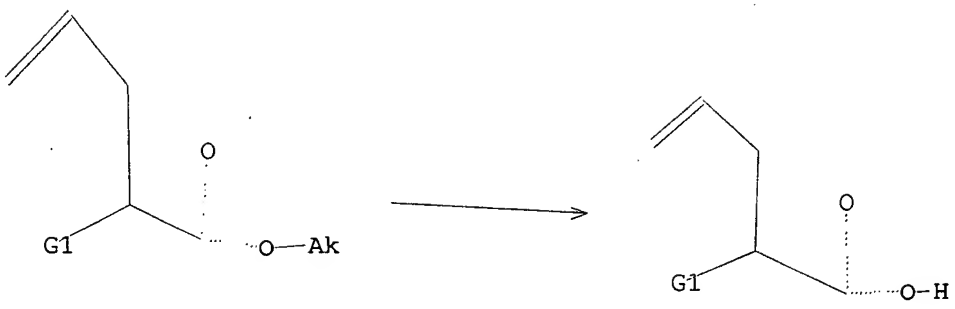



```
   1
 Ak

  Cb2
G1 [@1],[@2]

Structure attributes must be viewed using STN Express query preparation.

=> d l3
L3 HAS NO ANSWERS
L3               STR
```



Ak[1]

Cb[2]

G1 [@1],[@2]

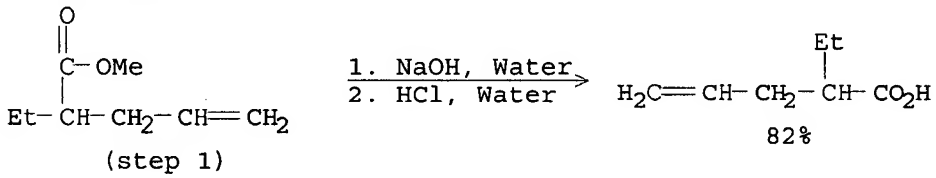
Structure attributes must be viewed using STN Express query preparation.

=> d scan

L8 27 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Syntheses of 20'-deoxyvinblastine, 20'-deoxyleurosidine, 20'-deoxyvincovaline, 20'-epi-20'-deoxyvincovaline, and 20'-deoxyvincristine and its 20'-epimer through racemic and enantioselectively generated intermediates. New syntheses of D/E-cis- and trans-Ψ-vincadifformines and D/E-cis- and -trans-20-epi-Ψ-vincadifformines

RX(31) OF 363

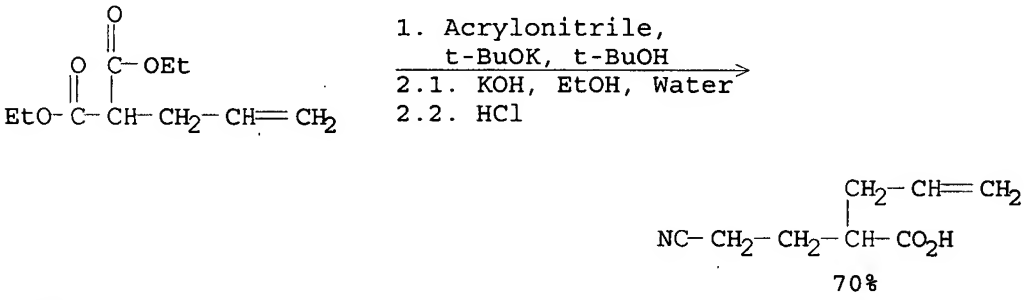


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):26

L8 27 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Asymmetric synthesis of 5- and 6-membered lactones from cyclic substrates bearing a C2-chiral auxiliary

RX(86) OF 104 - 3 STEPS

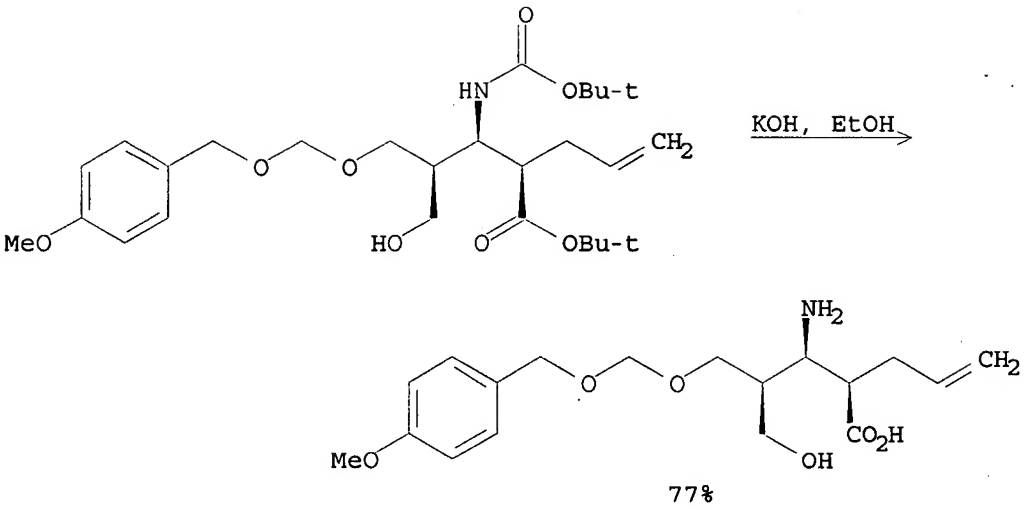


NOTE: 3) thermal

L8 27 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Asymmetric synthesis of protected α-alkyl β-amino δ-hydroxy esters by stereocontrolled elaboration of THYM

RX(11) OF 103

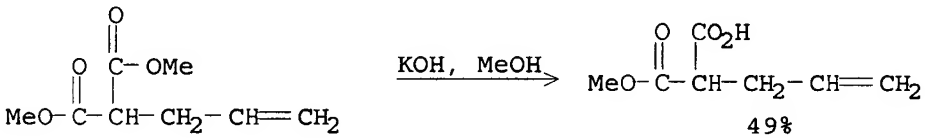


77%

L8 27 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Sulfur-mediated radical cyclization reactions on solid support

RX(6) OF 64

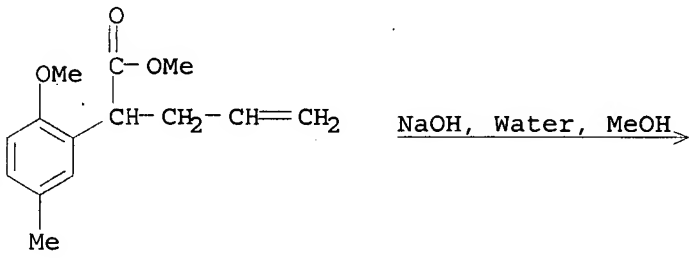


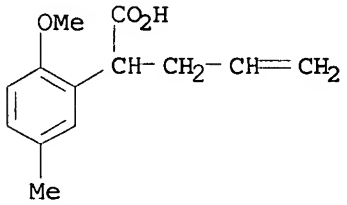
49%

L8 27 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Formal total synthesis of (±)-herbertene-1,13-diol and (±)-α-herbertenol via Ireland ester Claisen rearrangement and RCM reaction sequence

RX(6) OF 74



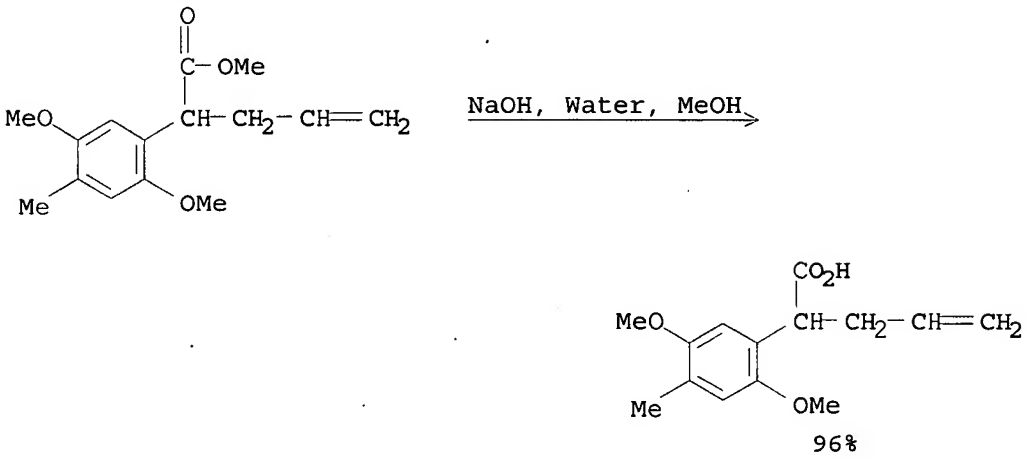


95%

L8 27 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI The first total synthesis of (±)-lagopodin A

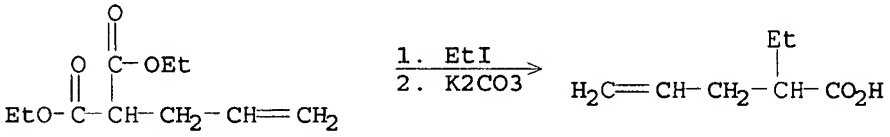
RX(15) OF 226



L8 27 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Synthesis of δ-lactones. V. Synthesis of 3-alkyl δ-lactones

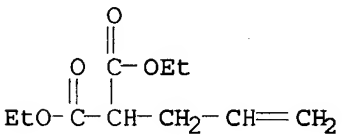
RX(40) OF 72 - 2 STEPS



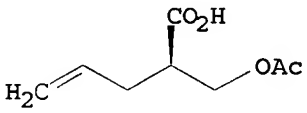
L8 27 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Preparative bioorganic chemistry. XI. Preparation of the enantiomers of paraconic acid employing lipase-mediated asymmetric hydrolysis of prochiral diacetates as the key step

RX(32) OF 53 - 4 STEPS



1.1. LiAlH4, Et2O
1.2. NaOH, Water
2. Ac2O, Pyridine
3.1. Ortho-Gynol, Water, Me2CO
3.2. Lipase, NaOH, Water
4. Me2CO



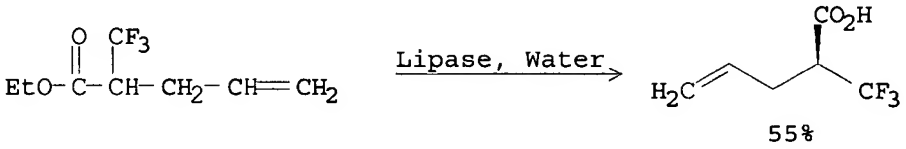
82%

NOTE: 3) lipase MY, 4) Jones' reagent

L8 27 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Synthesis of enantiomerically enriched α-trifluoromethylated acids, esters and ketones

RX(2) OF 6

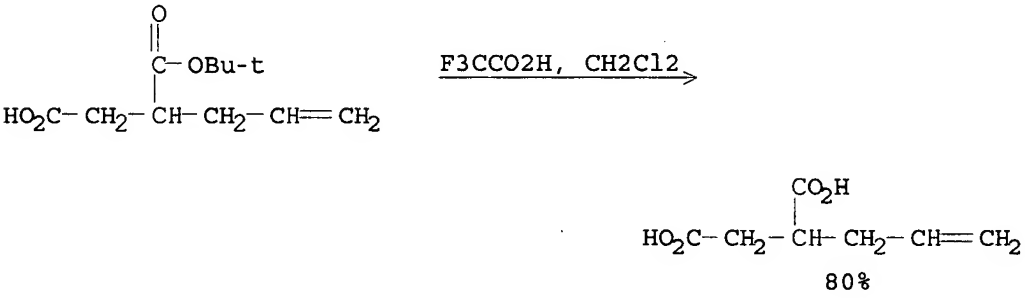


NOTE: enzymic, stereoselective

L8 27 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Synthesis of monosubstituted succinic acids from tert-butyl succinate

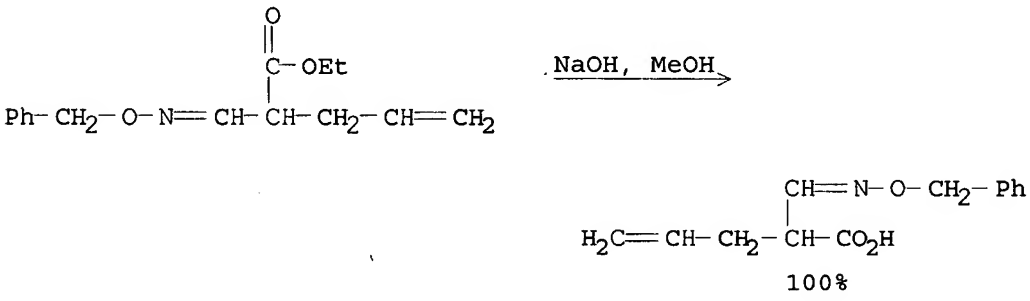
RX(11) OF 42



L8 27 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Structure-activity relationships of the peptide deformylase inhibitor BB-3497: modification of the methylene spacer and the P1' side chain

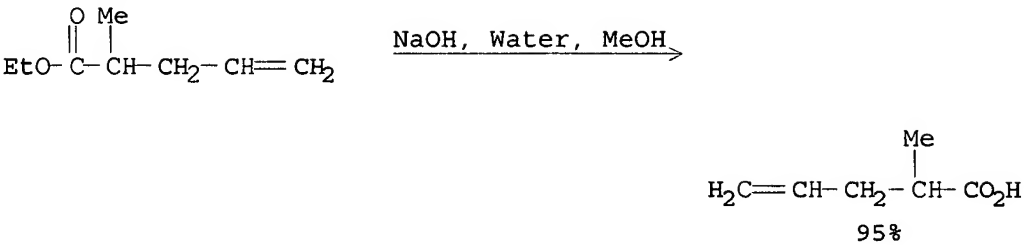
RX(49) OF 653



L8 27 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Construction of vicinal quaternary carbon atoms by Ireland ester Claisen rearrangement: total synthesis of (±)-herbertenolide, (±)-herberteneacetal, (±)-herbertene-1,14-diol and (±)-herbertene-1,15-diol

RX(4) OF 116

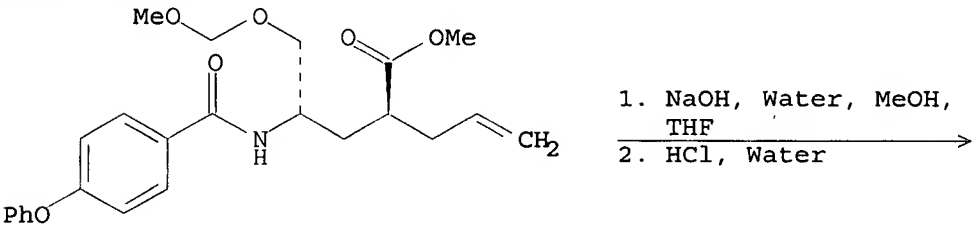


95%

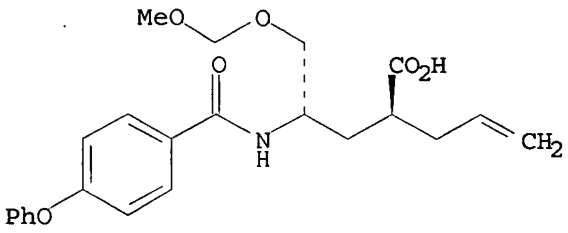
L8 27 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Design and synthesis of an orally active matrix metalloproteinase inhibitor

RX(27) OF 341



(step 1)

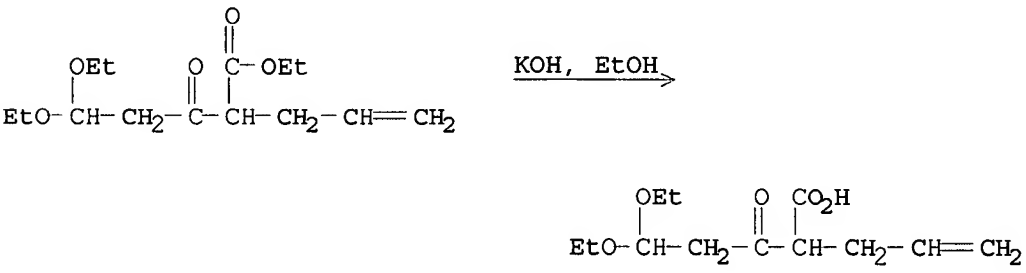


85%

L8 27 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Enol ethers. XVI. Synthesis of 4-hydroxy-2H-pyran-2-ones

RX(13) OF 67

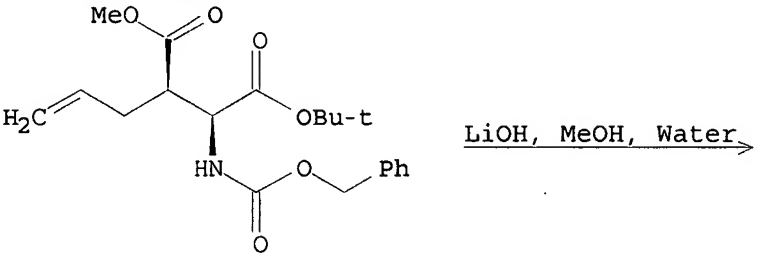


K

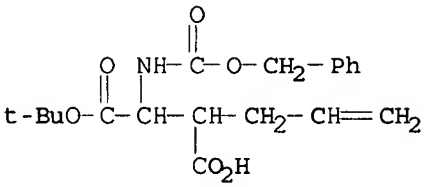
L8 27 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Asymmetric amino acid synthesis: preparation of the β anion derived from aspartic acid

RX(16) OF 66



LiOH, MeOH, Water

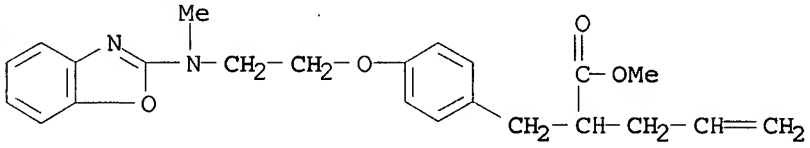


stereoisomers

L8 27 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

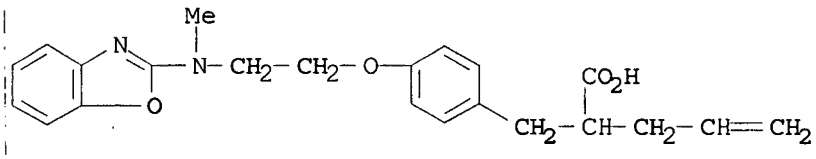
TI Preparation of [(benzoxazolylamino)alkoxy]phenylalkanoates and analogs as hypoglycemics

RX(1) OF 63



(step 1)

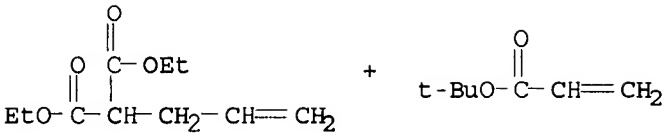
1. NaOH, Water, MeOH
2. HCl, Water



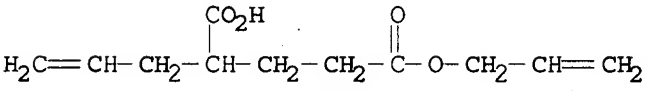
L8 27 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Design of a new macrocyclic sulfonamide peptidomimetics and synthesis of the precursors

RX(13) OF 13 - 4 STEPS



1.1. NaH, Hexane
2.1. EtOH
2.2. KOH, Water
3. Ac2O
4.1. Allyl alcohol, NaH, THF
4.2. THF



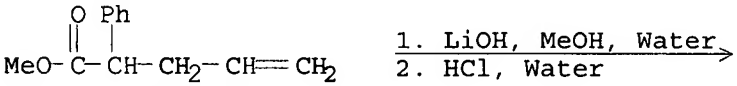
83%

NOTE: 2) reflux, 3) 100.degree., 4) controlled temp.

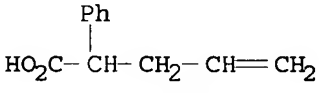
L8 27 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Synthesis and structure-antifungal activity relationships of 3-aryl-5-alkyl-2,5-dihydrofuran-2-ones and their carbanalogues: further refinement of tentative pharmacophore group

RX(24) OF 314



(step 1)

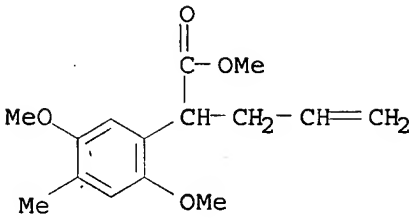


100%

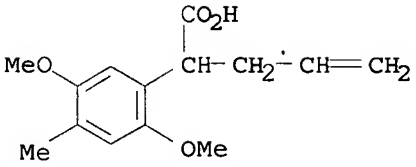
L8 27 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI The first total synthesis of a bioactive metabolite, a spirobenzofuran isolated from the fungi Acremonium sp. HKI 0230

RX(3) OF 117



NaOH, Water, MeOH



96%

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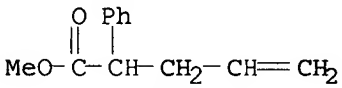
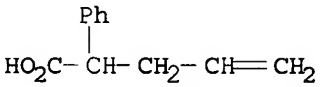
TI Room Temperature Hydroamination of N-Alkenyl Ureas Catalyzed by a Gold(I) N-Heterocyclic Carbene Complex

RX(10) OF 57



(step 1)

1. KOH, Water, MeOH, THF
2. HCl, Water

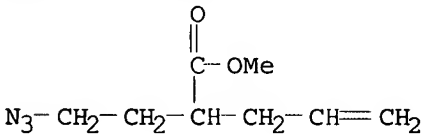


92%

L8 27 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

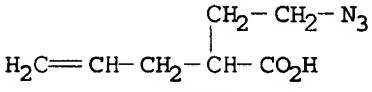
TI Synthesis and reactivity of methyl γ-azidobutyrates and ethyl δ-azidovalerates and of the corresponding acid chlorides as useful reagents for the aminoalkylation

RX(13) OF 198



(step 1)

1. NaOH, Water, MeOH
2. HCl, Water



89%

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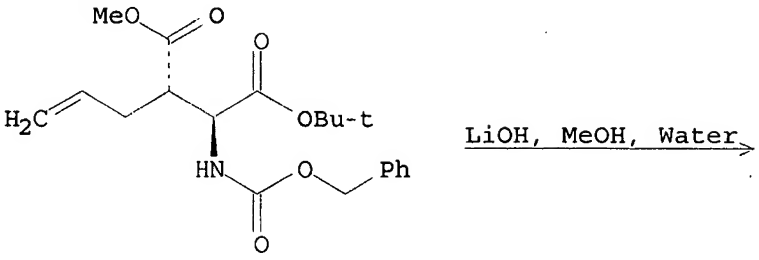
TI Non-proteinogenic amino acid synthesis. The β-anion derived from

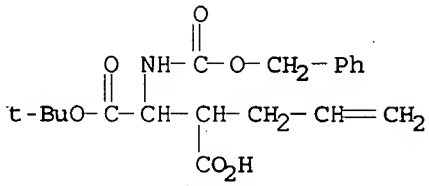
aspartic acid, and its application to α-amino acid synthesis

RX(11) OF 42



LiOH, MeOH, Water

stereoisomers



stereoisomers

NOTE: 57% overall

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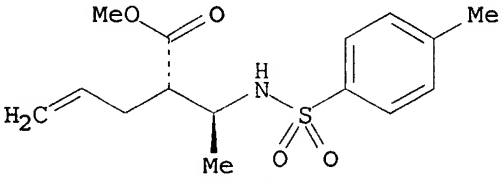
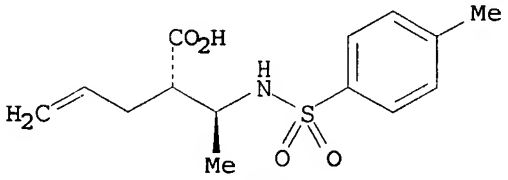
TI Stereoselective synthesis of enantiomerically pure 4,5-disubstituted pyrrolidinones from β-amino esters

RX(8) OF 41



(step 1)

1. NaOH, MeOH
2. HCl
3. AcOEt



96%

NOTE: STEREOSELECTIVE

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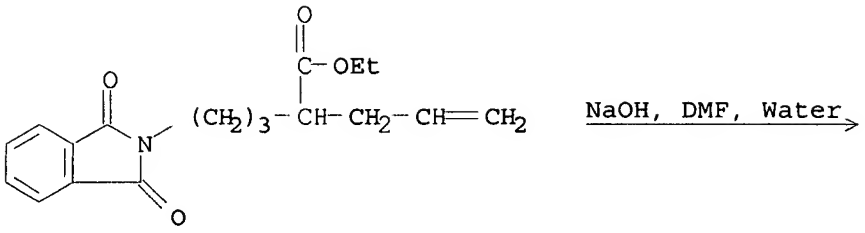
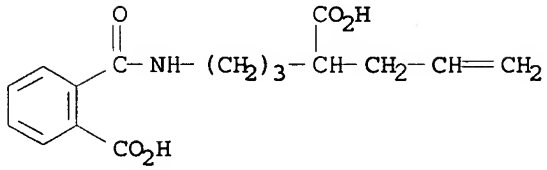
TI 2-(3-Aminopropyl)-4-pentenoic acid as a bio-compatible/cleavable linker for solid-phase organic synthesis

RX(3) OF 17

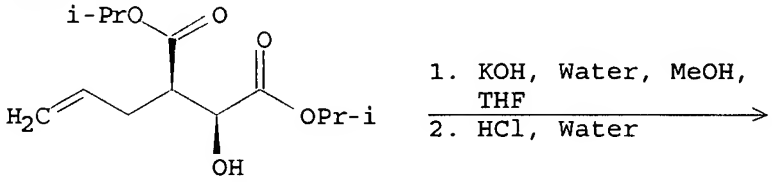




L8 27 ANSWERS CASREACT COPYRIGHT 2007 ACS on STN

TI Strategy in Inhibition of Cathepsin B, A Target in Tumor Invasion and Metastasis

RX(2) OF 118



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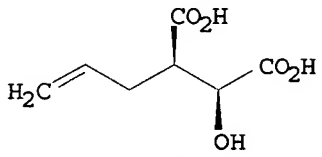

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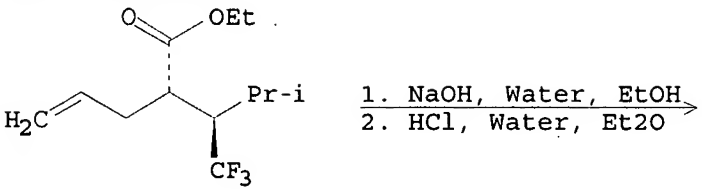
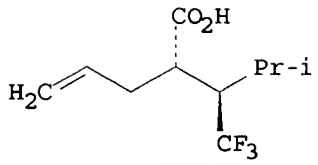
TI The effect of fluoromethyl groups on the diastereoselectivity in the electrophilic alkylation

RX(29) OF 224



(step 1)



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TI Pesticidal aromatic and alicyclic substituted acetates

RX(1) OF 12

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FULL ESTIMATED COST	16.05	131.97

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146:45449 Room Temperature Hydroamination of N-Alkenyl Ureas Catalyzed by a Gold(I) N-Heterocyclic Carbene Complex. Bender, Christopher F.; Widenhoefer, Ross A. (P. M. Gross Chemical Laboratory, Duke University, Durham, NC, 27708-0346, USA). Organic Letters, 8(23), 5303-5305 (English) 2006. CODEN: ORLEF7. ISSN: 1523-7060. Publisher: American Chemical Society.
TI Room Temperature Hydroamination of N-Alkenyl Ureas Catalyzed by a Gold(I) N-Heterocyclic Carbene Complex

L8 ANSWER 2 OF 27 CASREACT COPYRIGHT 2007 ACS on STN
145:369251 Design and synthesis of an orally active matrix metalloproteinase inhibitor. Yamamoto, Shingo; Nakatani, Shingo; Ikura, Masahiro; Sugiura, Tsuneyuki; Nishita, Yoshitaka; Itadani, Satoshi; Ogawa, Koji; Ohno, Hiroyuki; Takahashi, Kanji; Nakai, Hisao; Toda, Masaaki (Minase Research Institute, Ono Pharmaceutical Co., Ltd, 3-1-1 Sakurai, Shimamoto, Mishima, Osaka, 618-8585, Japan). Bioorganic & Medicinal Chemistry, 14(18), 6383-6403 (English) 2006. CODEN: BMECEP. ISSN: 0968-0896. Publisher: Elsevier B.V..
TI Design and synthesis of an orally active matrix metalloproteinase inhibitor

L8 ANSWER 3 OF 27 CASREACT COPYRIGHT 2007 ACS on STN
144:292896 The first total synthesis of (±)-lagopodin A. Srikrishna, A.; Vasantha Lakshmi, B.; Ravikumar, P. C. (Department of Organic Chemistry, Indian Institute of Science, Bangalore, 560 012, India). Tetrahedron Letters, 47(8), 1277-1281 (English) 2006. CODEN: TELEAY. ISSN: 0040-4039. Publisher: Elsevier B.V..
TI The first total synthesis of (±)-lagopodin A

L8 ANSWER 4 OF 27 CASREACT COPYRIGHT 2007 ACS on STN
144:191718 The effect of fluoromethyl groups on the diastereoselectivity in the electrophilic alkylation. Tamura, Kenji; Yamazaki, Takashi; Kitazume, Tomoya; Kubota, Toshio (Graduate School of Bioscience and Bioengineering, Tokyo Institute of Technology, Midori-ku, Yokohama, 226-8501, Japan). Journal of Fluorine Chemistry, 126(6), 918-930 (English) 2005. CODEN: JFLCAR. ISSN: 0022-1139. Publisher: Elsevier B.V..
TI The effect of fluoromethyl groups on the diastereoselectivity in the electrophilic alkylation

L8 ANSWER 5 OF 27 CASREACT COPYRIGHT 2007 ACS on STN
143:422180 The first total synthesis of a bioactive metabolite, a spirobenzofuran isolated from the fungi Acremonium sp. HKI 0230. Srikrishna, A.; Lakshmi, B. Vasantha (Department of Organic Chemistry,

Indian Institute of Science, Bangalore, 560012, India). Tetrahedron Letters, 46(41), 7029-7031 (English) 2005. CODEN: TELEAY. ISSN: 0040-4039. Publisher: Elsevier B.V..
TI The first total synthesis of a bioactive metabolite, a spirobenzofuran isolated from the fungi Acremonium sp. HKI 0230

L8 ANSWER 6 OF 27 CASREACT COPYRIGHT 2007 ACS on STN
143:212028 Construction of vicinal quaternary carbon atoms by Ireland ester Claisen rearrangement: total synthesis of (±)-herbertenolide, (±)-herberteneacetal, (±)-herbertene-1,14-diol and (±)-herbertene-1,15-diol. Srikrishna, A.; Vasantha Lakshmi, B. (Department of Organic Chemistry, Indian Institute of Science, Bangalore, 560012, India). Tetrahedron Letters, 46(29), 4879-4881 (English) 2005. CODEN: TELEAY. ISSN: 0040-4039. Publisher: Elsevier B.V..
TI Construction of vicinal quaternary carbon atoms by Ireland ester Claisen rearrangement: total synthesis of (±)-herbertenolide, (±)-herberteneacetal, (±)-herbertene-1,14-diol and (±)-herbertene-1,15-diol

L8 ANSWER 7 OF 27 CASREACT COPYRIGHT 2007 ACS on STN
143:133546 Formal total synthesis of (±)-herbertene-1,13-diol and (±)-α-herbertenol via Ireland ester Claisen rearrangement and RCM reaction sequence. Srikrishna, A.; Lakshmi, B. Vasantha (Department of Organic Chemistry, Indian Institute of Science, Bangalore, 560012, India). Synlett (7), 1173-1175 (English) 2005. CODEN: SYNLES. ISSN: 0936-5214. Publisher: Georg Thieme Verlag.
TI Formal total synthesis of (±)-herbertene-1,13-diol and (±)-α-herbertenol via Ireland ester Claisen rearrangement and RCM reaction sequence

L8 ANSWER 8 OF 27 CASREACT COPYRIGHT 2007 ACS on STN
141:270996 Strategy in Inhibition of Cathepsin B, A Target in Tumor Invasion and Metastasis. Lim, In Taek; Meroueh, Samy O.; Lee, Mijoon; Heeg, Mary Jane; Mobashery, Shahriar (Department of Chemistry and Biochemistry and Walther Cancer Research Center, University of Notre Dame, Notre Dame, IN, 46556, USA). Journal of the American Chemical Society, 126(33), 10271-10277 (English) 2004. CODEN: JACSAT. ISSN: 0002-7863. Publisher: American Chemical Society.
TI Strategy in Inhibition of Cathepsin B, A Target in Tumor Invasion and Metastasis

L8 ANSWER 9 OF 27 CASREACT COPYRIGHT 2007 ACS on STN
139:345312 Synthesis and structure-antifungal activity relationships of 3-aryl-5-alkyl-2,5-dihydrofuran-2-ones and their carbanalogues: further refinement of tentative pharmacophore group. Pour, Milan; Spulak, Marcel; Balsanek, Vojtech; Kunes, Jiri; Kubanova, Petra; Buchta, Vladimir (Faculty of Pharmacy, Department of Inorganic and Organic Chemistry, Laboratory of Structure and Interactions of Biologically Active Molecules, Charles University, Hradec Kralove, CZ-500 05, Czech Rep.). Bioorganic & Medicinal Chemistry, 11(13), 2843-2866 (English) 2003. CODEN: BMECEP. ISSN: 0968-0896. Publisher: Elsevier Science Ltd..
TI Synthesis and structure-antifungal activity relationships of 3-aryl-5-alkyl-2,5-dihydrofuran-2-ones and their carbanalogues: further refinement of tentative pharmacophore group

L8 ANSWER 10 OF 27 CASREACT COPYRIGHT 2007 ACS on STN
139:285636 Structure-activity relationships of the peptide deformylase inhibitor BB-3497: modification of the methylene spacer and the P1' side chain. Davies, Stephen J.; Ayscough, Andrew P.; Beckett, R. Paul; Bragg,

Ryan A.; Clements, John M.; Doel, Sheila; Grew, Christine; Launchbury, Steven B.; Perkins, Gemma M.; Pratt, Lisa M.; Smith, Helen K.; Spavold, Zoe M.; Thomas, S. Wayne; Todd, Richard S.; Whittaker, Mark (British Biotech Pharmaceuticals Limited, Oxford, OX4 6LY, UK). Bioorganic & Medicinal Chemistry Letters, 13(16), 2709-2713 (English) 2003. CODEN: BMCLE8. ISSN: 0960-894X. Publisher: Elsevier Science B.V..
TI Structure-activity relationships of the peptide deformylase inhibitor BB-3497: modification of the methylene spacer and the P1' side chain

L8 ANSWER 11 OF 27 CASREACT COPYRIGHT 2007 ACS on STN
138:385079 Sulfur-mediated radical cyclization reactions on solid support. Harrowven, David C.; May, Peter J.; Bradley, Mark (Department of Chemistry, The University of Southampton, Southampton, SO17 1BJ, UK). Tetrahedron Letters, Volume Date 2003, 44(3), 503-506 (English) 2002. CODEN: TELEAY. ISSN: 0040-4039. Publisher: Elsevier Science Ltd..
TI Sulfur-mediated radical cyclization reactions on solid support

L8 ANSWER 12 OF 27 CASREACT COPYRIGHT 2007 ACS on STN
137:294931 2-(3-Aminopropyl)-4-pentenoic acid as a bio-compatible/cleavable linker for solid-phase organic synthesis. Guo, Mao-Jun; Varady, Laszlo (Applications Development, ArQule Inc., Woburn, MA, 01801, USA). Tetrahedron Letters, 43(20), 3677-3680 (English) 2002. CODEN: TELEAY. ISSN: 0040-4039. Publisher: Elsevier Science Ltd..
TI 2-(3-Aminopropyl)-4-pentenoic acid as a bio-compatible/cleavable linker for solid-phase organic synthesis

L8 ANSWER 13 OF 27 CASREACT COPYRIGHT 2007 ACS on STN
136:340952 Design of a new macrocyclic sulfonamide peptidomimetics and synthesis of the precursors. Zhao, Bao-xiang; Blechert, Siegfried (School of Chemistry and Chemical Engineering, Shandong University, Jinan, 250100, Peop. Rep. China). Gaodeng Xuexiao Huaxue Xuebao, 22(12), 2045-2047 (Chinese) 2001. CODEN: KTHPDM. ISSN: 0251-0790. Publisher: Gaodeng Jiaoyu Chubanshe.
TI Design of a new macrocyclic sulfonamide peptidomimetics and synthesis of the precursors

L8 ANSWER 14 OF 27 CASREACT COPYRIGHT 2007 ACS on STN
134:4683 Synthesis of monosubstituted succinic acids from tert-butyl succinate. Bergmeier, Stephen C.; Ismail, Khadiga A. (Division of Medicinal Chemistry and Pharmacognosy, College of Pharmacy, The Ohio State University, Columbus, OH, 43210-1291, USA). Synthesis (10), 1369-1371 (English) 2000. CODEN: SYNTBF. ISSN: 0039-7881. Publisher: Georg Thieme Verlag.
TI Synthesis of monosubstituted succinic acids from tert-butyl succinate

L8 ANSWER 15 OF 27 CASREACT COPYRIGHT 2007 ACS on STN
133:120606 Asymmetric synthesis of protected α-alkyl β-amino δ-hydroxy esters by stereocontrolled elaboration of THYM. Guanti, Giuseppe; Moro, Alberto; Narisano, Enrica (Dip. Chim. Chim. Ind., Univ. Genova, Genoa, I-16146, Italy). Tetrahedron Letters, 41(17), 3203-3207 (English) 2000. CODEN: TELEAY. ISSN: 0040-4039. Publisher: Elsevier Science Ltd..
TI Asymmetric synthesis of protected α-alkyl β-amino δ-hydroxy esters by stereocontrolled elaboration of THYM

L8 ANSWER 16 OF 27 CASREACT COPYRIGHT 2007 ACS on STN
132:207722 Stereoselective synthesis of enantiomerically pure 4,5-disubstituted pyrrolidinones from β-amino esters. Wang, Jianbo;

Hou, Yihua; Wu, Peng; Qu, Zhaohui; Chan, Albert S. C. (Department of Chemistry, Peking University, Beijing, 100871, Peop. Rep. China). Tetrahedron: Asymmetry, 10(23), 4553-4561 (English) 1999. CODEN: TASYE3. ISSN: 0957-4166. Publisher: Elsevier Science Ltd..
TI Stereoselective synthesis of enantiomerically pure 4,5-disubstituted pyrrolidinones from β-amino esters

L8 ANSWER 17 OF 27 CASREACT COPYRIGHT 2007 ACS on STN
122:314541 Preparation of [(benzoxazolylamino)alkoxy]phenylalkanoates and analogs as hypoglycemics. Rami, Harshad Kantilal (Smithkline Beecham PLC, UK). PCT Int. Appl. WO 9503288 A1 19950202, 38 pp. DESIGNATED STATES: W: JP, US; RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1994-EP2029 19940620. PRIORITY: GB 1993-15148 19930722.
TI Preparation of [(benzoxazolylamino)alkoxy]phenylalkanoates and analogs as hypoglycemics

L8 ANSWER 18 OF 27 CASREACT COPYRIGHT 2007 ACS on STN
118:124038 Synthesis of enantiomerically enriched α-trifluoromethylated acids, esters and ketones. Watanabe, Shoji; Shimada, Yoshiaki; Kitazume, Tomoya; Yamazaki, Takashi (Fac. Eng., Chiba Univ., Chiba, 263, Japan). Journal of Fluorine Chemistry, 59(2), 249-56 (English) 1992. CODEN: JFLCAR. ISSN: 0022-1139.
TI Synthesis of enantiomerically enriched α-trifluoromethylated acids, esters and ketones

L8 ANSWER 19 OF 27 CASREACT COPYRIGHT 2007 ACS on STN
114:101618 Asymmetric synthesis of 5- and 6-membered lactones from cyclic substrates bearing a C2-chiral auxiliary. Yamamoto, Yukio; Sakamoto, Akio; Nishioka, Takaaki; Oda, Junichi; Fukazawa, Yoshimasa (College of Lib. Arts Sci., Kyoto Univ., Kyoto, 606, Japan). Journal of Organic Chemistry, 56(3), 1112-19 (English) 1991. CODEN: JOCEAH. ISSN: 0022-3263.
TI Asymmetric synthesis of 5- and 6-membered lactones from cyclic substrates bearing a C2-chiral auxiliary

L8 ANSWER 20 OF 27 CASREACT COPYRIGHT 2007 ACS on STN
113:24454 Non-proteinogenic amino acid synthesis. The β-anion derived from aspartic acid, and its application to α-amino acid synthesis. Baldwin, Jack E.; Moloney, Mark G.; North, Michael (Dyson Perrins Lab., Univ. Oxford, Oxford, OX1 3QY, UK). Tetrahedron, 45(19), 6309-18 (English) 1989. CODEN: TETRAB. ISSN: 0040-4020.
TI Non-proteinogenic amino acid synthesis. The β-anion derived from aspartic acid, and its application to α-amino acid synthesis

L8 ANSWER 21 OF 27 CASREACT COPYRIGHT 2007 ACS on STN
112:7865 Asymmetric amino acid synthesis: preparation of the β anion derived from aspartic acid. Baldwin, Jack E.; Moloney, Mark G.; North, Michael (Dyson Perrins Lab., Univ. Oxford, Oxford, OX1 3QY, UK). Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (4), 833-4 (English) 1989. CODEN: JCPRB4. ISSN: 0300-922X.
TI Asymmetric amino acid synthesis: preparation of the β anion derived from aspartic acid

L8 ANSWER 22 OF 27 CASREACT COPYRIGHT 2007 ACS on STN
111:214336 Preparative bioorganic chemistry. XI. Preparation of the enantiomers of paraconic acid employing lipase-mediated asymmetric

hydrolysis of prochiral diacetates as the key step. Mori, Kenji; Chiba, Naoki (Dep. Agric. Chem., Univ. Tokyo, Tokyo, 113, Japan). Liebigs Annalen der Chemie (10), 957-62 (English) 1989. CODEN: LACHDL. ISSN: 0170-2041.

TI Preparative bioorganic chemistry. XI. Preparation of the enantiomers of paraconic acid employing lipase-mediated asymmetric hydrolysis of prochiral diacetates as the key step

L8 ANSWER 23 OF 27 CASREACT COPYRIGHT 2007 ACS on STN

111:58131 Syntheses of 20'-deoxyvinblastine, 20'-deoxyleurosidine, 20'-deoxyvincovaline, 20'-epi-20'-deoxyvincovaline, and 20'-deoxyvincristine and its 20'-epimer through racemic and enantioselectively generated intermediates. New syntheses of D/E-cis- and trans-Ψ-vincadifformines and D/E-cis- and -trans-20-epi-Ψ-vincadifformines. Kuehne, Martin E.; Bornmann, William G. (Dep. Chem., Univ. Vermont, Burlington, VT, 05405, USA). Journal of Organic Chemistry, 54(14), 3407-20 (English) 1989. CODEN: JOCEAH. ISSN: 0022-3263.

TI Syntheses of 20'-deoxyvinblastine, 20'-deoxyleurosidine, 20'-deoxyvincovaline, 20'-epi-20'-deoxyvincovaline, and 20'-deoxyvincristine and its 20'-epimer through racemic and enantioselectively generated intermediates. New syntheses of D/E-cis- and trans-Ψ-vincadifformines and D/E-cis- and -trans-20-epi-Ψ-vincadifformines

L8 ANSWER 24 OF 27 CASREACT COPYRIGHT 2007 ACS on STN

108:167246 Synthesis and reactivity of methyl γ-azidobutyrates and ethyl δ-azidovalerates and of the corresponding acid chlorides as useful reagents for the aminoalkylation. Khoukhi, N.; Vaultier, M.; Carrie, R. (Groupe Physicochim. Struct., Univ. Rennes I, Rennes, 35042, Fr.). Tetrahedron, 43(8), 1811-22 (English) 1987. CODEN: TETRAB. ISSN: 0040-4020.

TI Synthesis and reactivity of methyl γ-azidobutyrates and ethyl δ-azidovalerates and of the corresponding acid chlorides as useful reagents for the aminoalkylation

L8 ANSWER 25 OF 27 CASREACT COPYRIGHT 2007 ACS on STN

102:184947 Enol ethers. XVI. Synthesis of 4-hydroxy-2H-pyran-2-ones. Effenberger, Franz; Ziegler, Thomas; Schoenwaelder, Karl Heinz (Inst. Org. Chem., Univ. Stuttgart, Stuttgart, 7000/80, Fed. Rep. Ger.). Chemische Berichte, 118(2), 741-52 (German) 1985. CODEN: CHBEAM. ISSN: 0009-2940.

TI Enol ethers. XVI. Synthesis of 4-hydroxy-2H-pyran-2-ones

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85:32383 Synthesis of δ-lactones. V. Synthesis of 3-alkyl δ-lactones. Kurata, Kumiko; Tanaka, Shigeru; Takahashi, Kiyoshi (Meiji Pharm. Coll., Tanashi, Japan). Chemical & Pharmaceutical Bulletin, 24(3), 538-40 (French) 1976. CODEN: CPBTAL. ISSN: 0009-2363.

TI Synthesis of δ-lactones. V. Synthesis of 3-alkyl δ-lactones

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80:120746 Pesticidal aromatic and alicyclic substituted acetates. (Sumitomo Chemical Co., Ltd.). Ger. Offen. DE 2335347 19740214, 176 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1973-2335347 19730711.

TI Pesticidal aromatic and alicyclic substituted acetates

=> log hold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION

FULL ESTIMATED COST 30.96 163.05

SESSION WILL BE HELD FOR 120 MINUTES
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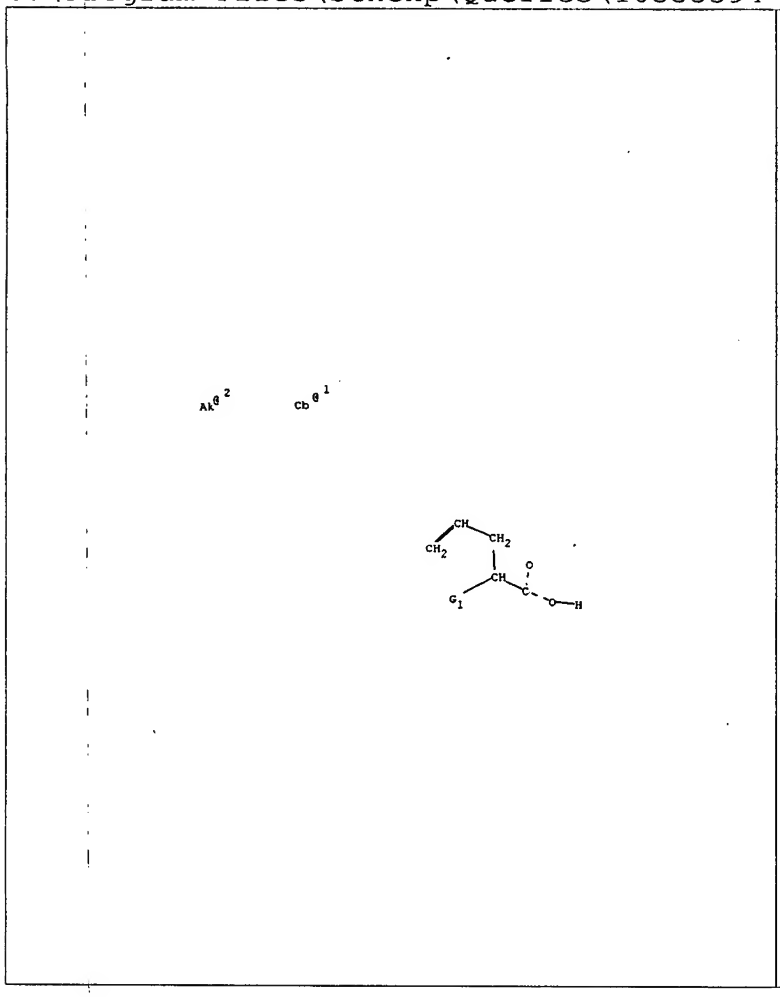

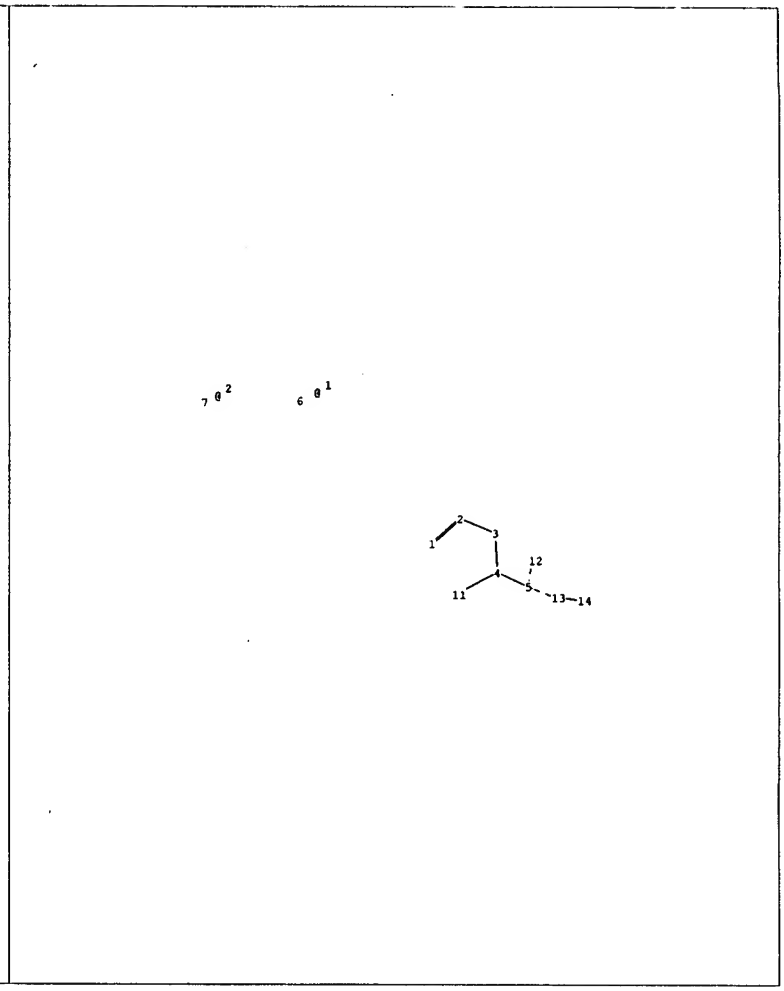

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chain bonds :
1-2 2-3 3-4 4-5 4-11 5-12 5-13 13-14
exact/norm bonds :
2-3 3-4 4-5 4-11 5-12 5-13
exact bonds :
1-2 13-14

G1:[*1],[*2]

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:Atom 7:CLASS 11:CLASS
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Generic attributes :
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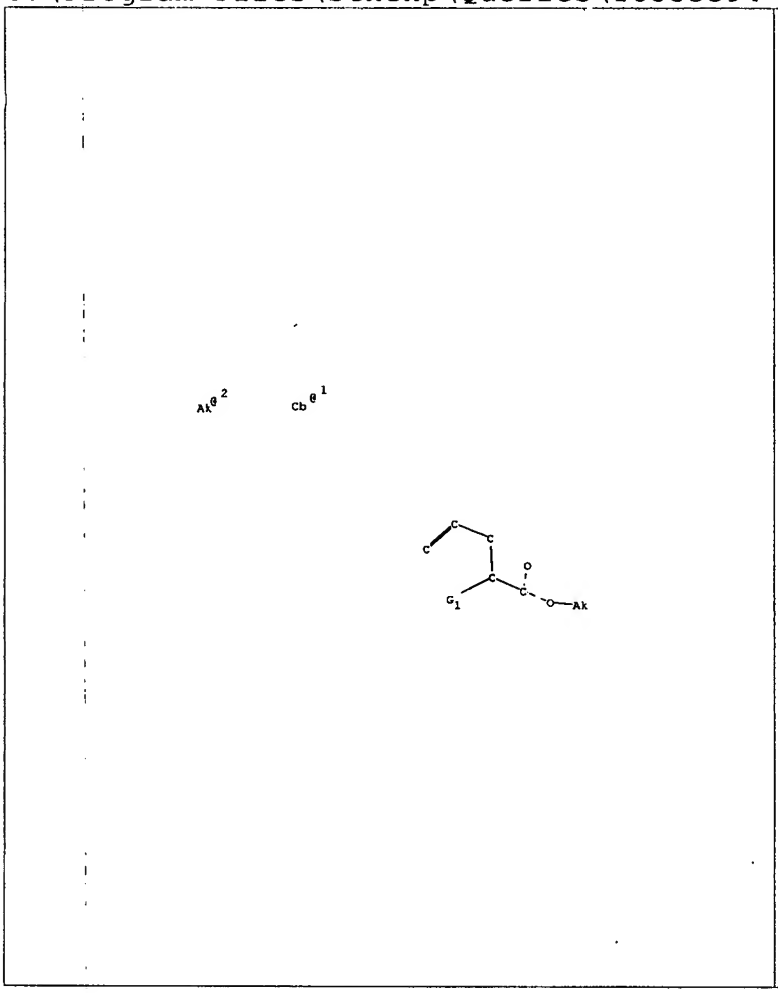

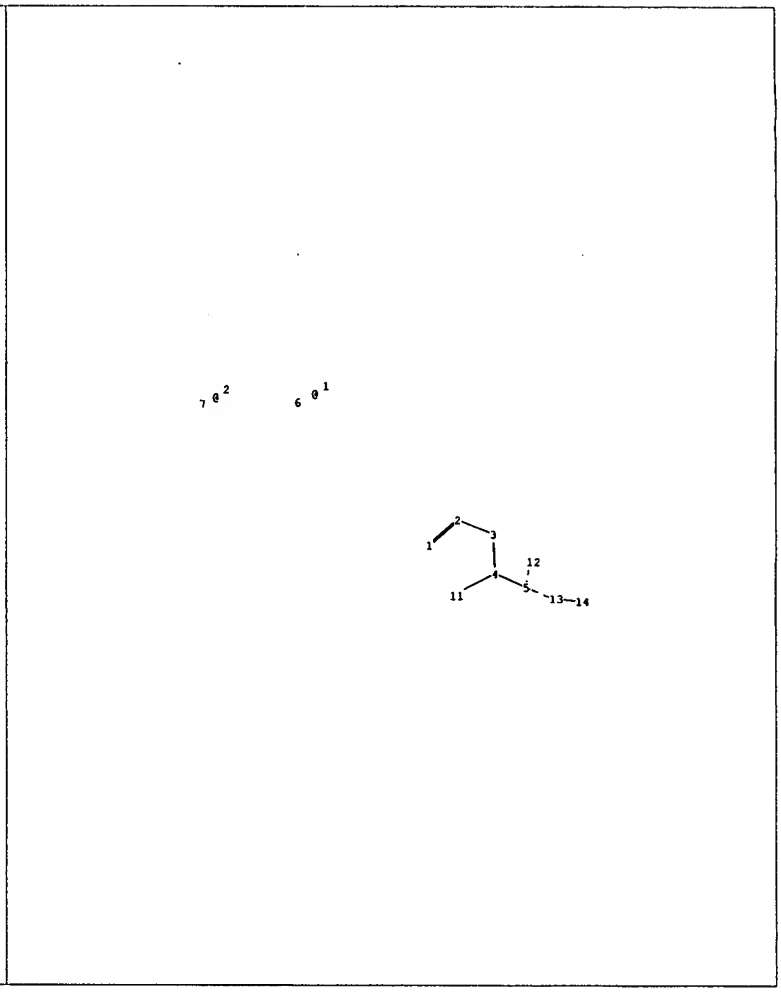

chain nodes :
1 2 3 4 5 6 7 11 12 13 14
chain bonds :
1-2 2-3 3-4 4-5 4-11 5-12 5-13 13-14
exact/norm bonds :
2-3 3-4 4-5 4-11 5-12 5-13 13-14
exact bonds :
1-2

G1:[*1],[*2]

Match level :
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